1-benzylpyrazole

Other names:	1-(phenylmethyl)-1H-pyrazole 1-benzyl-1H-pyrazole 1H-pyrazole, 1-(phenylmethyl)- N-benzylpyrazole pyrazole, 1-benzyl-
Inchi:	InChI=1S/C10H10N2/c1-2-5-10(6-3-1)9-12-8-4-7-11-12/h1-8H,9H2
InchiKey:	AKQAJYLKBCWJBV-UHFFFAOYSA-N
Formula:	C10H10N2
SMILES:	c1ccc(Cn2cccn2)cc1
Mol. weight [g/mol]:	158.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	1.931		Crippen Method
mcvol	128.500	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	1.47e-03	kPa	298.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	4.30e-03	kPa	310.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	6.15e-03	kPa	314.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	8.82e-03	kPa	318.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.01	kPa	322.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.02	kPa	326.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.02	kPa	326.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.02	kPa	330.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.03	kPa	334.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.04	kPa	338.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.06	kPa	342.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.07	kPa	346.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.10	kPa	350.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods

pvap	0.12	kPa	354.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods
pvap	0.16	kPa	358.20	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	382.00	K	0.60	Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Benchmark properties of pyrazole derivatives as a potential liquid organic hydrogen carrier: Evaluation of thermochemical data with complementary experimental and computational methods:	https://www.doi.org/10.1016/j.jct.2018.07.020

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tbp:	Boiling point at given pressure

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