

Benzene, 1-methoxy-2,4-bis(1-methyl-1-phenylethyl)-

Inchi:	InChI=1S/C25H28O/c1-24(2,19-12-8-6-9-13-19)21-16-17-23(26-5)22(18-21)25(3,4)20-14
InchiKey:	IKXRTMLXIDVXBX-UHFFFAOYSA-N
Formula:	C25H28O
SMILES:	COc1ccc(C(C)(C)c2ccccc2)cc1C(C)(C)c1ccccc1
Mol. weight [g/mol]:	344.49
CAS:	1262783-05-0

Physical Properties

Property code	Value	Unit	Source
gf	378.27	kJ/mol	Joback Method
hf	-22.40	kJ/mol	Joback Method
hfus	28.21	kJ/mol	Joback Method
hvap	79.21	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	6.347		Crippen Method
mcvol	297.700	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	2459.20		NIST Webbook
tb	877.36	K	Joback Method
tc	1131.62	K	Joback Method
tf	502.88	K	Joback Method
vc	1.107	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.02	J/molxK	877.36	Joback Method
cpg	937.62	J/molxK	919.74	Joback Method
cpg	954.72	J/molxK	962.11	Joback Method
cpg	970.49	J/molxK	1004.49	Joback Method
cpg	985.13	J/molxK	1046.87	Joback Method
cpg	998.81	J/molxK	1089.24	Joback Method
cpg	1011.72	J/molxK	1131.62	Joback Method
dvisc	0.0004099	Paxs	502.88	Joback Method

dvisc	0.0002001	Paxs	565.29	Joback Method
dvisc	0.0001127	Paxs	627.71	Joback Method
dvisc	0.0000704	Paxs	690.12	Joback Method
dvisc	0.0000475	Paxs	752.53	Joback Method
dvisc	0.0000341	Paxs	814.95	Joback Method
dvisc	0.0000256	Paxs	877.36	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1262783050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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