

Benzamide, pentafluoro-N-nonyl-

Inchi:	InChI=1S/C16H20F5NO/c1-2-3-4-5-6-7-8-9-22-16(23)10-11(17)13(19)15(21)14(20)12(10)
InchiKey:	JXYQQTHELUBGTI-UHFFFAOYSA-N
Formula:	C16H20F5NO
SMILES:	CCCCCCCCNC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	337.33

Physical Properties

Property code	Value	Unit	Source
gf	-865.48	kJ/mol	Joback Method
hf	-1234.05	kJ/mol	Joback Method
hfus	51.39	kJ/mol	Joback Method
hvap	65.89	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	4.862		Crippen Method
mvol	232.940	ml/mol	McGowan Method
pc	1427.22	kPa	Joback Method
rinpol	1996.00		NIST Webbook
rinpol	1996.00		NIST Webbook
tb	717.45	K	Joback Method
tc	891.18	K	Joback Method
tf	464.64	K	Joback Method
vc	0.955	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.27	J/mol×K	717.45	Joback Method
cpg	679.96	J/mol×K	746.41	Joback Method
cpg	692.96	J/mol×K	775.36	Joback Method
cpg	705.30	J/mol×K	804.32	Joback Method
cpg	716.98	J/mol×K	833.27	Joback Method
cpg	728.02	J/mol×K	862.23	Joback Method
cpg	738.44	J/mol×K	891.18	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U407945&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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