

Benzamide, pentafluoro-N-octadecyl-

Inchi:	InChI=1S/C25H38F5NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-31-25(32)19-20
InchiKey:	ZXCFCZHTRXIARH-UHFFFAOYSA-N
Formula:	C25H38F5NO
SMILES:	CCCCCCCCCCCCCCCCCNC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	463.57

Physical Properties

Property code	Value	Unit	Source
gf	-789.70	kJ/mol	Joback Method
hf	-1419.81	kJ/mol	Joback Method
hfus	74.70	kJ/mol	Joback Method
hvap	85.93	kJ/mol	Joback Method
log10ws	-10.59		Crippen Method
logp	8.373		Crippen Method
mvol	359.750	ml/mol	McGowan Method
pc	811.22	kPa	Joback Method
rinpol	2899.00		NIST Webbook
tb	923.37	K	Joback Method
tc	1135.76	K	Joback Method
tf	566.07	K	Joback Method
vc	1.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1197.49	J/mol×K	923.37	Joback Method
cpg	1216.33	J/mol×K	958.77	Joback Method
cpg	1233.87	J/mol×K	994.17	Joback Method
cpg	1250.16	J/mol×K	1029.56	Joback Method
cpg	1265.25	J/mol×K	1064.96	Joback Method
cpg	1279.22	J/mol×K	1100.36	Joback Method
cpg	1292.11	J/mol×K	1135.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407951&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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