Benzamide, pentafluoro-N-hexadecyl-

Inchi: InChI=1S/C23H34F5NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-29-23(30)17-18(24)20
InchiKey: QOOUHTXRPVWVEG-UHFFFAOYSA-N
Formula: C23H34F5NO
SMILES: CCCCCCCCCCCCCCCCCNC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 435.51

Physical Properties

Property code	Value	Unit	Source
gf	-806.54	kJ/mol	Joback Method
hf	-1378.53	kJ/mol	Joback Method
hfus	69.52	kJ/mol	Joback Method
hvap	81.47	kJ/mol	Joback Method
log10ws	-9.75		Crippen Method
logp	7.593		Crippen Method
mcvol	331.570	ml/mol	McGowan Method
pc	907.79	kPa	Joback Method
rinpol	2690.00		NIST Webbook
rinpol	2690.00		NIST Webbook
tb	877.61	K	Joback Method
tc	1075.19	K	Joback Method
tf	543.53	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1073.89	J/mol×K	877.61	Joback Method
cpg	1091.38	J/mol×K	910.54	Joback Method
cpg	1107.77	J/mol×K	943.47	Joback Method
cpg	1123.10	J/mol×K	976.40	Joback Method
cpg	1137.41	J/mol×K	1009.33	Joback Method
cpg	1150.74	J/mol×K	1042.26	Joback Method
cpg	1163.13	J/mol×K	1075.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
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