2-Adamantylamine, N-heptafluorobutyryl-

Inchi: InChI=1S/C14H16F7NO/c15-12(16,13(17,18)14(19,20)21)11(23)22-10-8-2-6-1-7(4-8)5-9
InchiKey: SMVNJSTXQNLGSD-UHFFFAOYSA-N
Formula: C14H16F7NO
SMILES: O=C(NC1C2CC3CC(C2)CC1C3)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 347.27

Physical Properties

Property code	Value	Unit	Source
gf	-1172.95	kJ/mol	Joback Method
hf	-1618.86	kJ/mol	Joback Method
hfus	32.48	kJ/mol	Joback Method
hvap	49.63	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.760		Crippen Method
mcvol	199.480	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	624.11	K	Joback Method
tc	806.04	K	Joback Method
tf	403.34	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.59	J/mol×K	624.11	Joback Method
cpg	642.74	J/mol×K	654.43	Joback Method
cpg	658.65	J/mol×K	684.75	Joback Method
cpg	673.41	J/mol×K	715.08	Joback Method
cpg	687.14	J/mol×K	745.40	Joback Method
cpg	699.93	J/mol×K	775.72	Joback Method
cpg	711.89	J/mol×K	806.04	Joback Method

Sources

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=U374859&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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