2-Adamantylamine, N-trifluoroacetyl-

Inchi: InChI=1S/C12H16F3NO/c13-12(14,15)11(17)16-10-8-2-6-1-7(4-8)5-9(10)3-6/h6-10H,1-5
InchiKey: RNQNAVNYZPAYBC-UHFFFAOYSA-N
Formula: C12H16F3NO
SMILES: O=C(NC1C2CC3CC(C2)CC1C3)C(F)(F)F
Mol. weight [g/mol]: 247.26

Physical Properties

Property code	Value	Unit	Source
gf	-416.23	kJ/mol	Joback Method
hf	-775.64	kJ/mol	Joback Method
hfus	29.81	kJ/mol	Joback Method
hvap	51.03	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.490		Crippen Method
mcvol	164.220	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
tb	587.73	K	Joback Method
tc	786.67	K	Joback Method
tf	373.60	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.70	J/mol×K	587.73	Joback Method
cpg	500.81	J/mol×K	620.89	Joback Method
cpg	517.66	J/mol×K	654.04	Joback Method
cpg	533.34	J/mol×K	687.20	Joback Method
cpg	547.94	J/mol×K	720.36	Joback Method
cpg	561.55	J/mol×K	753.51	Joback Method
cpg	574.28	J/mol×K	786.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374750&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

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