N-(3,5-Dimethyl-1-adamantyl)trifluoroacetamide

Other names: 3,5-Dimethyladamantan-1-yl-trifluoroacetamine
3,5-Dimethyltricyclo[3.3.1.13,7]decan-1-trifluoroacetamine
Inchi: InChI=1S/C14H20F3NO/c1-11-3-9-4-12(2,6-11)8-13(5-9,7-11)18-10(19)14(15,16)17/h9H
InchiKey: PRMUEKWAUBTBRV-UHFFFAOYSA-N
Formula: C14H20F3NO
SMILES: CC12CC3CC(C)(C1)CC(NC(=O)C(F)(F)F)(C3)C2
Mol. weight [g/mol]: 275.31

Physical Properties

Property code	Value	Unit	Source
gf	-408.15	kJ/mol	Joback Method
hf	-750.86	kJ/mol	Joback Method
hfus	15.02	kJ/mol	Joback Method
hvap	52.34	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.414		Crippen Method
mcvol	192.400	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	1484.00		NIST Webbook
tb	638.88	K	Joback Method
tc	853.93	K	Joback Method
tf	472.08	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.69	J/mol×K	638.88	Joback Method
cpg	595.23	J/mol×K	674.72	Joback Method
cpg	611.86	J/mol×K	710.56	Joback Method
cpg	627.97	J/mol×K	746.41	Joback Method
cpg	643.93	J/mol×K	782.25	Joback Method
cpg	660.13	J/mol×K	818.09	Joback Method
cpg	676.95	J/mol×K	853.93	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=U373419&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