Trifluoroacetamide, N-(1-methylheptyl)

Inchi: InChI=1S/C11H20F3NO/c1-3-4-5-6-7-8-9(2)15-10(16)11(12,13)14/h9H,3-8H2,1-2H3,(H,1
InchiKey: AJHVEAHKNSGFMO-UHFFFAOYSA-N
Formula: C11H20F3NO
SMILES: CCCCCCCC(C)NC(=O)C(F)(F)F
Mol. weight [g/mol]: 239.28

Physical Properties

Property code	Value	Unit	Source
gf	-581.82	kJ/mol	Joback Method
hf	-931.84	kJ/mol	Joback Method
hfus	29.25	kJ/mol	Joback Method
hvap	49.13	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.414		Crippen Method
mcvol	182.710	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	1161.00		NIST Webbook
tb	549.26	K	Joback Method
tc	713.59	K	Joback Method
tf	305.51	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.18	J/mol×K	549.26	Joback Method
cpg	484.70	J/mol×K	576.65	Joback Method
cpg	498.52	J/mol×K	604.04	Joback Method
cpg	511.67	J/mol×K	631.42	Joback Method
cpg	524.17	J/mol×K	658.81	Joback Method
cpg	536.04	J/mol×K	686.20	Joback Method
cpg	547.32	J/mol×K	713.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R74088&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