N-Trifluoroacetyl-2-octylamine

Other names: Trifluoroacetamide, N-(1-methylhexyl)
Inchi: InChI=1S/C10H18F3NO/c1-3-4-5-6-7-8(2)14-9(15)10(11,12)13/h8H,3-7H2,1-2H3,(H,14,1
InchiKey: PCWNWQNPOLREHV-UHFFFAOYSA-N
Formula: C10H18F3NO
SMILES: CCCCCCC(C)NC(=O)C(F)(F)F
Mol. weight [g/mol]: 225.25
CAS: 96592-05-1

Physical Properties

Property code	Value	Unit	Source
gf	-590.24	kJ/mol	Joback Method
hf	-911.20	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	46.90	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.024		Crippen Method
mcvol	168.620	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	1065.00		NIST Webbook
rinpol	1065.00		NIST Webbook
tb	526.38	K	Joback Method
tc	691.55	K	Joback Method
tf	294.24	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.74	J/mol×K	526.38	Joback Method
cpg	435.65	J/mol×K	553.91	Joback Method
cpg	448.89	J/mol×K	581.44	Joback Method
cpg	461.48	J/mol×K	608.97	Joback Method
cpg	473.44	J/mol×K	636.49	Joback Method
cpg	484.80	J/mol×K	664.02	Joback Method

cpg	495.59	J/mol×K	691.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96592051&Units=SI

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