Pentafluoropropanamide, N,N-dihexyl-

Inchi: InChI=1S/C15H26F5NO/c1-3-5-7-9-11-21(12-10-8-6-4-2)13(22)14(16,17)15(18,19)20/h3
InchiKey: VZKAXEAQMWMMLH-UHFFFAOYSA-N
Formula: C15H26F5NO
SMILES: CCCCCCN(CCCCCC)C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 331.37

Physical Properties

Property code	Value	Unit	Source
gf	-911.09	kJ/mol	Joback Method
hf	-1396.03	kJ/mol	Joback Method
hfus	39.80	kJ/mol	Joback Method
hvap	51.10	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	5.173		Crippen Method
mcvol	242.610	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	1534.00		NIST Webbook
rinpol	1534.00		NIST Webbook
tb	598.80	K	Joback Method
tc	751.52	K	Joback Method
tf	349.00	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.00	J/mol×K	598.80	Joback Method
cpg	691.38	J/mol×K	624.25	Joback Method
cpg	706.95	J/mol×K	649.71	Joback Method
cpg	721.74	J/mol×K	675.16	Joback Method
cpg	735.80	J/mol×K	700.61	Joback Method
cpg	749.17	J/mol×K	726.07	Joback Method
cpg	761.87	J/mol×K	751.52	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=U308511&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