Heptafluorobutanamide, N,N-diheptyl-

Inchi: InChI=1S/C18H30F7NO/c1-3-5-7-9-11-13-26(14-12-10-8-6-4-2)15(27)16(19,20)17(21,22
InchiKey: KSUKSKFLNBADIC-UHFFFAOYSA-N
Formula: C18H30F7NO
SMILES: CCCCCCCN(CCCCCCC)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 409.43

Physical Properties

Property code	Value	Unit	Source
gf	-1272.61	kJ/mol	Joback Method
hf	-1858.92	kJ/mol	Joback Method
hfus	46.31	kJ/mol	Joback Method
hvap	54.84	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	6.589		Crippen Method
mcvol	288.420	ml/mol	McGowan Method
pc	1012.30	kPa	Joback Method
rinpol	1734.00		NIST Webbook
tb	662.75	K	Joback Method
tc	816.99	K	Joback Method
tf	386.41	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.54	J/mol×K	662.75	Joback Method
cpg	877.66	J/mol×K	688.46	Joback Method
cpg	893.90	J/mol×K	714.16	Joback Method
cpg	909.29	J/mol×K	739.87	Joback Method
cpg	923.89	J/mol×K	765.58	Joback Method
cpg	937.75	J/mol×K	791.28	Joback Method
cpg	950.91	J/mol×K	816.99	Joback Method

Sources

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=U308274&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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