N,N-di-n-Butylheptafluorobutyramide

Other names: Heptafluorobutanamide, N,N-dibutyl-
Inchi: InChI=1S/C12H18F7NO/c1-3-5-7-20(8-6-4-2)9(21)10(13,14)11(15,16)12(17,18)19/h3-8H
InchiKey: SSLBWWFVNPTUPO-UHFFFAOYSA-N
Formula: C12H18F7NO
SMILES: CCCCN(CCCC)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 325.27
CAS: 120219-46-7

Physical Properties

Property code	Value	Unit	Source
gf	-1323.13	kJ/mol	Joback Method
hf	-1735.08	kJ/mol	Joback Method
hfus	30.77	kJ/mol	Joback Method
hvap	41.49	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.248		Crippen Method
mcvol	203.880	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	1203.00		NIST Webbook
tb	525.47	K	Joback Method
tc	672.48	K	Joback Method
tf	318.79	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.61	J/mol×K	525.47	Joback Method
cpg	552.42	J/mol×K	549.97	Joback Method
cpg	566.42	J/mol×K	574.47	Joback Method
cpg	579.67	J/mol×K	598.98	Joback Method
cpg	592.18	J/mol×K	623.48	Joback Method
cpg	604.00	J/mol×K	647.98	Joback Method
cpg	615.16	J/mol×K	672.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120219467&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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