6-Amino-1-hexanol, N,O-bis(heptafluorobutyryl)-

Inchi: InChI=1S/C14H13F14NO3/c15-9(16,11(19,20)13(23,24)25)7(30)29-5-3-1-2-4-6-32-8(31)

InchiKey: AIEANBIIGMZCRV-UHFFFAOYSA-N

Formula: C14H13F14NO3

SMILES: O=C(NCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 509.24

Physical Properties

Property code	Value	Unit	Source
gf	-2916.75	kJ/mol	Joback Method
hf	-3434.24	kJ/mol	Joback Method
hfus	40.14	kJ/mol	Joback Method
hvap	49.88	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.872		Crippen Method
mcvol	251.890	ml/mol	McGowan Method
pc	1144.44	kPa	Joback Method
rinpol	1421.00		NIST Webbook
tb	670.45	K	Joback Method
tc	823.46	K	Joback Method
tf	445.07	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.17	J/mol×K	670.45	Joback Method
cpg	789.93	J/mol×K	695.95	Joback Method
cpg	800.85	J/mol×K	721.45	Joback Method
cpg	811.01	J/mol×K	746.96	Joback Method
cpg	820.45	J/mol×K	772.46	Joback Method
cpg	829.24	J/mol×K	797.96	Joback Method
cpg	837.43	J/mol×K	823.46	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=U375563&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