6-Bromohexanoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C11H13BrF8O2/c12-5-3-1-2-4-7(21)22-6-9(15,16)11(19,20)10(17,18)8(13)14/h

InchiKey: DWUJWKXBFFVPBY-UHFFFAOYSA-N

Formula: C11H13BrF8O2

SMILES: O=C(CCCCCBr)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 409.11

Physical Properties

Property code	Value	Unit	Source
gf	-1730.26	kJ/mol	Joback Method
hf	-2089.25	kJ/mol	Joback Method
hfus	31.19	kJ/mol	Joback Method
hvap	44.86	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.656		Crippen Method
mcvol	204.950	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	1507.00		NIST Webbook
rinpol	1507.00		NIST Webbook
tb	577.56	K	Joback Method
tc	734.87	K	Joback Method
tf	342.67	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.04	J/mol×K	577.56	Joback Method
cpg	549.16	J/mol×K	603.78	Joback Method
cpg	560.55	J/mol×K	630.00	Joback Method
cpg	571.25	J/mol×K	656.21	Joback Method
cpg	581.28	J/mol×K	682.43	Joback Method
cpg	590.71	J/mol×K	708.65	Joback Method
cpg	599.55	J/mol×K	734.87	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=U354711&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