4-Bromobutyric acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C9H9BrF8O2/c10-3-1-2-5(19)20-4-7(13,14)9(17,18)8(15,16)6(11)12/h6H,1-4H

InchiKey: GWXQJRHYHUDUGU-UHFFFAOYSA-N

Formula: C9H9BrF8O2

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

Mol. weight [g/mol]: 381.06

Physical Properties

Property code	Value	Unit	Source
gf	-1747.10	kJ/mol	Joback Method
hf	-2047.97	kJ/mol	Joback Method
hfus	26.01	kJ/mol	Joback Method
hvap	40.41	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.876		Crippen Method
mcvol	176.770	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	1272.00		NIST Webbook
rinpol	1272.00		NIST Webbook
tb	531.80	K	Joback Method
tc	689.55	K	Joback Method
tf	320.13	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.99	J/mol×K	531.80	Joback Method
cpg	453.08	J/mol×K	558.09	Joback Method
cpg	463.46	J/mol×K	584.38	Joback Method
cpg	473.17	J/mol×K	610.68	Joback Method
cpg	482.25	J/mol×K	636.97	Joback Method
cpg	490.72	J/mol×K	663.26	Joback Method
cpg	498.64	J/mol×K	689.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354682&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

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