Heptafluorobutyric acid, 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C10H3BrF8O2/c11-5-3-4(12)1-2-6(5)21-7(20)8(13,14)9(15,16)10(17,18)19/h1-

InchiKey: WIFDCTLCGYQDNW-UHFFFAOYSA-N

Formula: C10H3BrF8O2

SMILES: O=C(Oc1ccc(F)cc1Br)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 387.02

Physical Properties

Property code	Value	Unit	Source
gf	-1643.09	kJ/mol	Joback Method
hf	-1849.74	kJ/mol	Joback Method
hfus	25.39	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.327		Crippen Method
mcvol	167.100	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	850.00		NIST Webbook
rinpol	850.00		NIST Webbook
tb	591.76	K	Joback Method
tc	778.47	K	Joback Method
tf	397.86	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.96	J/mol×K	591.76	Joback Method
cpg	422.33	J/mol×K	622.88	Joback Method
cpg	430.89	J/mol×K	654.00	Joback Method
cpg	438.69	J/mol×K	685.11	Joback Method
cpg	445.80	J/mol×K	716.23	Joback Method
cpg	452.27	J/mol×K	747.35	Joback Method
cpg	458.15	J/mol×K	778.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299083&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