Succinic acid, 2-bromo-4-fluorophenyl 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C14H9BrF8O4/c15-8-5-7(16)1-2-9(8)27-11(25)4-3-10(24)26-6-12(17,18)13(19,

InchiKey: JBNZMYHAFRGUMJ-UHFFFAOYSA-N

Formula: C14H9BrF8O4

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

Mol. weight [g/mol]: 473.11

Physical Properties

Property code	Value	Unit	Source
gf	-1843.33	kJ/mol	Joback Method
hf	-2177.10	kJ/mol	Joback Method
hfus	38.54	kJ/mol	Joback Method
hvap	64.68	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	4.650		Crippen Method
mcvol	230.900	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	1795.00		NIST Webbook
rinpol	1795.00		NIST Webbook
tb	759.57	K	Joback Method
tc	948.51	K	Joback Method
tf	515.10	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.40	J/mol×K	759.57	Joback Method
cpg	655.02	J/mol×K	791.06	Joback Method
cpg	663.87	J/mol×K	822.55	Joback Method
cpg	672.01	J/mol×K	854.04	Joback Method
cpg	679.49	J/mol×K	885.53	Joback Method
cpg	686.38	J/mol×K	917.02	Joback Method
cpg	692.72	J/mol×K	948.51	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=U358010&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