Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C15H10BrF9O4/c16-8-5-7(17)1-2-9(8)29-11(27)4-3-10(26)28-6-13(20,21)15(24

InchiKey: XNSNNFCMKUQTDQ-UHFFFAOYSA-N

Formula: C15H10BrF9O4

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

Mol. weight [g/mol]: 505.13

Physical Properties

Property code	Value	Unit	Source
gf	-2032.16	kJ/mol	Joback Method
hf	-2399.13	kJ/mol	Joback Method
hfus	40.68	kJ/mol	Joback Method
hvap	65.70	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	4.988		Crippen Method
mcvol	246.760	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
tb	781.28	K	Joback Method
tc	968.12	K	Joback Method
tf	511.96	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.60	J/mol×K	781.28	Joback Method
cpg	716.44	J/mol×K	812.42	Joback Method
cpg	725.49	J/mol×K	843.56	Joback Method
cpg	733.83	J/mol×K	874.70	Joback Method
cpg	741.50	J/mol×K	905.84	Joback Method
cpg	748.58	J/mol×K	936.98	Joback Method
cpg	755.10	J/mol×K	968.12	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=U389762&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume