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

Inchi: InChI=1S/C16H13BrF8O5/c1-28-10-6-8(17)2-3-9(10)30-12(27)5-4-11(26)29-7-14(20,21)1

InchiKey: GKDOVCRFBNWPIE-UHFFFAOYSA-N

Formula: C16H13BrF8O5

SMILES: COc1cc(Br)ccc1OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 517.16

Physical Properties

Property code	Value	Unit	Source
gf	-1933.93	kJ/mol	Joback Method
hf	-2355.88	kJ/mol	Joback Method
hfus	41.38	kJ/mol	Joback Method
hvap	71.15	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	4.857		Crippen Method
mcvol	264.950	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	2207.00		NIST Webbook
rinpol	2207.00		NIST Webbook
tb	827.31	K	Joback Method
tc	1020.70	K	Joback Method
tf	544.87	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.42	J/mol×K	827.31	Joback Method
cpg	788.70	J/mol×K	859.54	Joback Method
cpg	798.13	J/mol×K	891.77	Joback Method
cpg	806.76	J/mol×K	924.00	Joback Method
cpg	814.66	J/mol×K	956.24	Joback Method
cpg	821.87	J/mol×K	988.47	Joback Method
cpg	828.45	J/mol×K	1020.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390911&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