Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 1-bromo-3,3,3-trifluoroprop-2-yl ester

Inchi: InChI=1S/C12H10BrF11O4/c13-3-5(11(20,21)22)28-7(26)2-1-6(25)27-4-9(16,17)12(23,2

InchiKey: JITWADYAUSNCDE-UHFFFAOYSA-N

Formula: C12H10BrF11O4

SMILES: O=C(CCC(=O)OC(CBr)C(F)(F)F)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 507.09

Physical Properties

Property code	Value	Unit	Source
gf	-2539.79	kJ/mol	Joback Method
hf	-2957.05	kJ/mol	Joback Method
hfus	34.87	kJ/mol	Joback Method
hvap	52.11	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.350		Crippen Method
mcvol	231.790	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpol	1463.00		NIST Webbook
tb	670.87	K	Joback Method
tc	831.99	K	Joback Method
tf	415.29	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.59	J/mol×K	670.87	Joback Method
cpg	669.99	J/mol×K	697.72	Joback Method
cpg	679.66	J/mol×K	724.58	Joback Method
cpg	688.65	J/mol×K	751.43	Joback Method
cpg	696.99	J/mol×K	778.29	Joback Method
cpg	704.74	J/mol×K	805.14	Joback Method
cpg	711.93	J/mol×K	831.99	Joback Method

Sources

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=U390820&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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