Succinic acid, 2-methylpent-3-yl 1-bromo-3,3,3-trifluoroprop-2-yl ester

Inchi: InChI=1S/C13H20BrF3O4/c1-4-9(8(2)3)20-11(18)5-6-12(19)21-10(7-14)13(15,16)17/h8-1

InchiKey: XETVBIJJHGAPBW-UHFFFAOYSA-N

Formula: C13H20BrF3O4

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

Mol. weight [g/mol]: 377.19

Physical Properties

Property code	Value	Unit	Source
gf	-983.85	kJ/mol	Joback Method
hf	-1387.84	kJ/mol	Joback Method
hfus	31.54	kJ/mol	Joback Method
hvap	64.37	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.613		Crippen Method
mcvol	231.720	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	1612.00		NIST Webbook
rinpol	1612.00		NIST Webbook
tb	708.84	K	Joback Method
tc	893.25	K	Joback Method
tf	399.58	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.54	J/mol×K	708.84	Joback Method
cpg	653.99	J/mol×K	739.58	Joback Method
cpg	666.65	J/mol×K	770.31	Joback Method
cpg	678.54	J/mol×K	801.05	Joback Method
cpg	689.68	J/mol×K	831.78	Joback Method
cpg	700.09	J/mol×K	862.52	Joback Method
cpg	709.80	J/mol×K	893.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390821&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

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