Succinic acid, 3-methylbut-2-en-1-yl 1-bromo-3,3,3-trifluoroprop-2-yl ester

Inchi: InChI=1S/C12H16BrF3O4/c1-8(2)5-6-19-10(17)3-4-11(18)20-9(7-13)12(14,15)16/h5,9H,3

InchiKey: BKGAOIMVEOTFFV-UHFFFAOYSA-N

Formula: C12H16BrF3O4

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

Mol. weight [g/mol]: 361.15

Physical Properties

Property code	Value	Unit	Source
gf	-915.72	kJ/mol	Joback Method
hf	-1249.21	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	62.96	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.145		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	690.88	K	Joback Method
tc	878.70	K	Joback Method
tf	399.27	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.20	J/mol×K	690.88	Joback Method
cpg	575.34	J/mol×K	722.18	Joback Method
cpg	586.75	J/mol×K	753.49	Joback Method
cpg	597.46	J/mol×K	784.79	Joback Method
cpg	607.52	J/mol×K	816.09	Joback Method
cpg	616.94	J/mol×K	847.40	Joback Method
cpg	625.76	J/mol×K	878.70	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=U390822&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