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

Inchi: InChI=1S/C19H30BrF3O4/c1-2-3-4-5-6-7-8-9-10-11-14-26-17(24)12-13-18(25)27-16(15-
InchiKey: GFDZYWQBXZVADT-ZHACJKMWSA-N
Formula: C19H30BrF3O4
SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)OC(CBr)C(F)(F)F
Mol. weight [g/mol]: 459.34

Physical Properties

Property code	Value	Unit	Source
gf	-848.23	kJ/mol	Joback Method
hf	-1383.90	kJ/mol	Joback Method
hfus	54.33	kJ/mol	Joback Method
hvap	78.46	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.876		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1159.29	kPa	Joback Method
rinpol	2358.00		NIST Webbook
rinpol	2358.00		NIST Webbook
tb	851.16	K	Joback Method
tc	1043.76	K	Joback Method
tf	492.12	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.49	J/mol×K	851.16	Joback Method
cpg	968.64	J/mol×K	883.26	Joback Method
cpg	982.86	J/mol×K	915.36	Joback Method
cpg	996.21	J/mol×K	947.46	Joback Method
cpg	1008.73	J/mol×K	979.56	Joback Method
cpg	1020.49	J/mol×K	1011.66	Joback Method
cpg	1031.52	J/mol×K	1043.76	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=U390835&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