Diethylmalonic acid, 1-bromo-3,3,3-trifluoroprop-2-yl tetradecyl ester

Inchi: InChI=1S/C24H42BrF3O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-31-21(29)23(5-2,6-3)2
InchiKey: USFSMDXQIURBKU-UHFFFAOYSA-N
Formula: C24H42BrF3O4
SMILES: CCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(CBr)C(F)(F)F
Mol. weight [g/mol]: 531.49

Physical Properties

Property code	Value	Unit	Source
gf	-883.51	kJ/mol	Joback Method
hf	-1613.07	kJ/mol	Joback Method
hfus	59.66	kJ/mol	Joback Method
hvap	88.33	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	7.906		Crippen Method
mcvol	386.710	ml/mol	McGowan Method
pc	840.16	kPa	Joback Method
rinpol	2544.00		NIST Webbook
tb	958.17	K	Joback Method
tc	1176.41	K	Joback Method
tf	555.97	K	Joback Method
vc	1.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.56	J/mol×K	958.17	Joback Method
cpg	1303.70	J/mol×K	994.54	Joback Method
cpg	1320.58	J/mol×K	1030.92	Joback Method
cpg	1336.31	J/mol×K	1067.29	Joback Method
cpg	1350.98	J/mol×K	1103.67	Joback Method
cpg	1364.70	J/mol×K	1140.04	Joback Method
cpg	1377.57	J/mol×K	1176.41	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=U370806&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