Dimethylmalonic acid, 1-bromo-3,3,3-trifluoroprop-2-yl hexyl ester

Inchi: InChI=1S/C14H22BrF3O4/c1-4-5-6-7-8-21-11(19)13(2,3)12(20)22-10(9-15)14(16,17)18/h

InchiKey: DZKNTSRXMPOANL-UHFFFAOYSA-N

Formula: C14H22BrF3O4

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

Mol. weight [g/mol]: 391.22

Physical Properties

Property code	Value	Unit	Source
gf	-967.71	kJ/mol	Joback Method
hf	-1406.67	kJ/mol	Joback Method
hfus	33.76	kJ/mol	Joback Method
hvap	66.07	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	4.005		Crippen Method
mcvol	245.810	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	1624.00		NIST Webbook
tb	729.37	K	Joback Method
tc	915.17	K	Joback Method
tf	443.27	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.01	J/mol×K	729.37	Joback Method
cpg	709.73	J/mol×K	760.34	Joback Method
cpg	722.60	J/mol×K	791.30	Joback Method
cpg	734.68	J/mol×K	822.27	Joback Method
cpg	745.98	J/mol×K	853.23	Joback Method
cpg	756.57	J/mol×K	884.20	Joback Method
cpg	766.47	J/mol×K	915.17	Joback Method

Sources

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=U361932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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