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

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

InchiKey: LISDAQXZDFIOQB-UHFFFAOYSA-N

Formula: C14H22BrF3O4

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

Mol. weight [g/mol]: 391.22

Physical Properties

Property code	Value	Unit	Source
gf	-970.15	kJ/mol	Joback Method
hf	-1411.95	kJ/mol	Joback Method
hfus	30.24	kJ/mol	Joback Method
hvap	65.69	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.861		Crippen Method
mcvol	245.810	ml/mol	McGowan Method
pc	1623.29	kPa	Joback Method
rinpol	1521.00		NIST Webbook
tb	728.93	K	Joback Method
tc	917.04	K	Joback Method
tf	428.27	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.55	J/mol×K	728.93	Joback Method
cpg	710.46	J/mol×K	760.28	Joback Method
cpg	723.49	J/mol×K	791.63	Joback Method
cpg	735.69	J/mol×K	822.98	Joback Method
cpg	747.10	J/mol×K	854.34	Joback Method
cpg	757.76	J/mol×K	885.69	Joback Method
cpg	767.71	J/mol×K	917.04	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=U370795&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