Dimethylmalonic acid, di(1-bromo-3,3,3-trifluoroprop-2-yl) ester

Inchi: InChI=1S/C11H12Br2F6O4/c1-9(2,7(20)22-5(3-12)10(14,15)16)8(21)23-6(4-13)11(17,18

InchiKey: SAIFPIKBRNLLGC-UHFFFAOYSA-N

Formula: C11H12Br2F6O4

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

Mol. weight [g/mol]: 482.01

Physical Properties

Property code	Value	Unit	Source
gf	-1562.68	kJ/mol	Joback Method
hf	-1920.78	kJ/mol	Joback Method
hfus	29.58	kJ/mol	Joback Method
hvap	61.70	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.751		Crippen Method
mcvol	226.350	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	1444.00		NIST Webbook
tb	721.03	K	Joback Method
tc	911.60	K	Joback Method
tf	458.45	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.35	J/mol×K	721.03	Joback Method
cpg	611.40	J/mol×K	752.79	Joback Method
cpg	620.68	J/mol×K	784.55	Joback Method
cpg	629.26	J/mol×K	816.32	Joback Method
cpg	637.18	J/mol×K	848.08	Joback Method
cpg	644.51	J/mol×K	879.84	Joback Method
cpg	651.30	J/mol×K	911.60	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=U361934&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