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

Inchi: InChI=1S/C8H9BrClF3O3/c1-7(2,5(10)14)6(15)16-4(3-9)8(11,12)13/h4H,3H2,1-2H3

InchiKey: FAIJPJUQKQBBPG-UHFFFAOYSA-N

Formula: C8H9BrClF3O3

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

Mol. weight [g/mol]: 325.51

Physical Properties

Property code	Value	Unit	Source
gf	-925.16	kJ/mol	Joback Method
hf	-1166.35	kJ/mol	Joback Method
hfus	21.23	kJ/mol	Joback Method
hvap	54.69	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.647		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	1196.00		NIST Webbook
rinpol	1196.00		NIST Webbook
tb	607.10	K	Joback Method
tc	807.93	K	Joback Method
tf	383.34	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.29	J/mol×K	607.10	Joback Method
cpg	402.20	J/mol×K	640.57	Joback Method
cpg	411.36	J/mol×K	674.04	Joback Method
cpg	419.79	J/mol×K	707.52	Joback Method
cpg	427.57	J/mol×K	740.99	Joback Method
cpg	434.73	J/mol×K	774.46	Joback Method
cpg	441.33	J/mol×K	807.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U361935&Units=SI

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