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

Inchi: InChI=1S/C10H13BrClF3O3/c1-3-9(4-2,7(12)16)8(17)18-6(5-11)10(13,14)15/h6H,3-5H2,

InchiKey: YCUHVTMPPPRDCK-UHFFFAOYSA-N

Formula: C10H13BrClF3O3

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

Mol. weight [g/mol]: 353.56

Physical Properties

Property code	Value	Unit	Source
gf	-908.32	kJ/mol	Joback Method
hf	-1207.63	kJ/mol	Joback Method
hfus	26.41	kJ/mol	Joback Method
hvap	59.14	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.427		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	1323.00		NIST Webbook
tb	652.86	K	Joback Method
tc	848.61	K	Joback Method
tf	405.88	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.12	J/mol×K	652.86	Joback Method
cpg	499.28	J/mol×K	685.49	Joback Method
cpg	509.66	J/mol×K	718.11	Joback Method
cpg	519.29	J/mol×K	750.74	Joback Method
cpg	528.24	J/mol×K	783.36	Joback Method
cpg	536.54	J/mol×K	815.99	Joback Method
cpg	544.26	J/mol×K	848.61	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=U370812&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