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

Inchi: InChI=1S/C12H18BrF3O4/c1-4-11(5-2,9(17)19-6-3)10(18)20-8(7-13)12(14,15)16/h8H,4-

InchiKey: SHELHCHMXZRKSG-UHFFFAOYSA-N

Formula: C12H18BrF3O4

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

Mol. weight [g/mol]: 363.17

Physical Properties

Property code	Value	Unit	Source
gf	-984.55	kJ/mol	Joback Method
hf	-1365.39	kJ/mol	Joback Method
hfus	28.58	kJ/mol	Joback Method
hvap	61.62	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.225		Crippen Method
mcvol	217.630	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	1405.00		NIST Webbook
tb	683.61	K	Joback Method
tc	870.94	K	Joback Method
tf	420.73	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.28	J/mol×K	683.61	Joback Method
cpg	602.17	J/mol×K	714.83	Joback Method
cpg	614.25	J/mol×K	746.05	Joback Method
cpg	625.57	J/mol×K	777.28	Joback Method
cpg	636.15	J/mol×K	808.50	Joback Method
cpg	646.04	J/mol×K	839.72	Joback Method
cpg	655.27	J/mol×K	870.94	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=U370793&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