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

Inchi: InChI=1S/C13H16Br2F6O4/c1-3-11(4-2,9(22)24-7(5-14)12(16,17)18)10(23)25-8(6-15)13

InchiKey: YTKUZSDIEUGPBV-UHFFFAOYSA-N

Formula: C13H16Br2F6O4

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

Mol. weight [g/mol]: 510.06

Physical Properties

Property code	Value	Unit	Source
gf	-1545.84	kJ/mol	Joback Method
hf	-1962.06	kJ/mol	Joback Method
hfus	34.76	kJ/mol	Joback Method
hvap	66.15	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.531		Crippen Method
mcvol	254.530	ml/mol	McGowan Method
pc	1689.34	kPa	Joback Method
rinpol	1561.00		NIST Webbook
tb	766.79	K	Joback Method
tc	956.48	K	Joback Method
tf	480.99	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.22	J/mol×K	766.79	Joback Method
cpg	717.14	J/mol×K	798.41	Joback Method
cpg	727.29	J/mol×K	830.02	Joback Method
cpg	736.72	J/mol×K	861.64	Joback Method
cpg	745.49	J/mol×K	893.25	Joback Method
cpg	753.67	J/mol×K	924.87	Joback Method
cpg	761.32	J/mol×K	956.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370811&Units=SI
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

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