Dimethylmalonic acid, di(2-bromo-4-fluorophenyl) ester

Inchi: InChI=1S/C17H12Br2F2O4/c1-17(2,15(22)24-13-5-3-9(20)7-11(13)18)16(23)25-14-6-4-1

InchiKey: RKMAWGRZJFHJKW-UHFFFAOYSA-N

Formula: C17H12Br2F2O4

SMILES: CC(C)(C(=O)Oc1ccc(F)cc1Br)C(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 478.08

Physical Properties

Property code	Value	Unit	Source
gf	-547.42	kJ/mol	Joback Method
hf	-804.94	kJ/mol	Joback Method
hfus	41.20	kJ/mol	Joback Method
hvap	88.89	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	5.027		Crippen Method
mcvol	256.290	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	2423.00		NIST Webbook
tb	941.85	K	Joback Method
tc	1187.66	K	Joback Method
tf	651.79	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.42	J/mol×K	941.85	Joback Method
cpg	692.46	J/mol×K	982.82	Joback Method
cpg	700.51	J/mol×K	1023.79	Joback Method
cpg	707.64	J/mol×K	1064.76	Joback Method
cpg	713.93	J/mol×K	1105.72	Joback Method
cpg	719.44	J/mol×K	1146.69	Joback Method
cpg	724.23	J/mol×K	1187.66	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=U361827&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