Diethylmalonic acid, monochloride, 4-bromophenyl ester

Inchi: InChI=1S/C13H14BrClO3/c1-3-13(4-2,11(15)16)12(17)18-10-7-5-9(14)6-8-10/h5-8H,3-4H

InchiKey: DDUBNKAPHZKMOV-UHFFFAOYSA-N

Formula: C13H14BrClO3

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 333.61

Physical Properties

Property code	Value	Unit	Source
gf	-196.25	kJ/mol	Joback Method
hf	-442.13	kJ/mol	Joback Method
hfus	29.53	kJ/mol	Joback Method
hvap	72.90	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.926		Crippen Method
mcvol	209.020	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook
tb	759.02	K	Joback Method
tc	994.69	K	Joback Method
tf	489.44	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.71	J/mol×K	759.02	Joback Method
cpg	536.61	J/mol×K	798.30	Joback Method
cpg	547.53	J/mol×K	837.58	Joback Method
cpg	557.54	J/mol×K	876.85	Joback Method
cpg	566.72	J/mol×K	916.13	Joback Method
cpg	575.11	J/mol×K	955.41	Joback Method
cpg	582.80	J/mol×K	994.69	Joback Method
dvisc	0.0008541	Pa×s	489.44	Joback Method

dvisc	0.0005255	Pa×s	534.37	Joback Method
dvisc	0.0003486	Pa×s	579.30	Joback Method
dvisc	0.0002453	Pa×s	624.23	Joback Method
dvisc	0.0001810	Pa×s	669.16	Joback Method
dvisc	0.0001387	Pa×s	714.09	Joback Method
dvisc	0.0001097	Pa×s	759.02	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=U369836&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
dvisc:	Dynamic viscosity
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