Diethylmalonic acid, monochloride, 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C14H16BrClO4/c1-4-14(5-2,12(16)17)13(18)20-10-7-6-9(15)8-11(10)19-3/h6-8

InchiKey: QIRIDLNLOMJESS-UHFFFAOYSA-N

Formula: C14H16BrClO4

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1ccc(Br)cc1OC

Mol. weight [g/mol]: 363.63

Physical Properties

Property code	Value	Unit	Source
gf	-302.46	kJ/mol	Joback Method
hf	-606.46	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	78.19	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.935		Crippen Method
mcvol	228.980	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	2130.00		NIST Webbook
tb	809.30	K	Joback Method
tc	1039.08	K	Joback Method
tf	535.46	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.29	J/mol×K	809.30	Joback Method
cpg	651.00	J/mol×K	1000.79	Joback Method
cpg	642.88	J/mol×K	962.49	Joback Method
cpg	633.89	J/mol×K	924.19	Joback Method
cpg	623.99	J/mol×K	885.89	Joback Method
cpg	613.14	J/mol×K	847.60	Joback Method
cpg	658.29	J/mol×K	1039.08	Joback Method
dvisc	0.0000712	Pa×s	809.30	Joback Method
dvisc	0.0000888	Pa×s	763.66	Joback Method

dvisc	0.0001140	Pa×s	718.02	Joback Method
dvisc	0.0001512	Pa×s	672.38	Joback Method
dvisc	0.0002091	Pa×s	626.74	Joback Method
dvisc	0.0003043	Pa×s	581.10	Joback Method
dvisc	0.0004719	Pa×s	535.46	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=U371166&Units=SI

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