Glutaric acid, 2,2-dichloroethyl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C14H15BrCl2O5/c1-20-11-7-9(15)5-6-10(11)22-14(19)4-2-3-13(18)21-8-12(16)

InchiKey: ZVYRBACTABEXIX-UHFFFAOYSA-N

Formula: C14H15BrCl2O5

SMILES: COc1cc(Br)ccc1OC(=O)CCCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 414.08

Physical Properties

Property code	Value	Unit	Source
gf	-424.67	kJ/mol	Joback Method
hf	-750.95	kJ/mol	Joback Method
hfus	42.20	kJ/mol	Joback Method
hvap	85.90	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.880		Crippen Method
mcvol	247.090	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	2622.00		NIST Webbook
rinpol	2622.00		NIST Webbook
tb	871.94	K	Joback Method
tc	1097.00	K	Joback Method
tf	570.19	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.28	J/mol×K	871.94	Joback Method
cpg	686.58	J/mol×K	1059.49	Joback Method
cpg	680.65	J/mol×K	1021.98	Joback Method
cpg	673.66	J/mol×K	984.47	Joback Method
cpg	665.60	J/mol×K	946.96	Joback Method
cpg	656.47	J/mol×K	909.45	Joback Method
cpg	691.43	J/mol×K	1097.00	Joback Method
dvisc	0.0000521	Pa×s	871.94	Joback Method

dvisc	0.0000647	Pa×s	821.65	Joback Method
dvisc	0.0000827	Pa×s	771.36	Joback Method
dvisc	0.0001093	Pa×s	721.07	Joback Method
dvisc	0.0001506	Pa×s	670.77	Joback Method
dvisc	0.0002186	Pa×s	620.48	Joback Method
dvisc	0.0003388	Pa×s	570.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393885&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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