Glutaric acid, 3-chlorophenyl 4-bromophenyl ester

Inchi: InChI=1S/C17H14BrClO4/c18-12-7-9-14(10-8-12)22-16(20)5-2-6-17(21)23-15-4-1-3-13(1

InchiKey: YKXMSYGQBWSFOH-UHFFFAOYSA-N

Formula: C17H14BrClO4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 397.65

Physical Properties

Property code	Value	Unit	Source
gf	-167.63	kJ/mol	Joback Method
hf	-423.10	kJ/mol	Joback Method
hfus	42.15	kJ/mol	Joback Method
hvap	88.44	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.784		Crippen Method
mcvol	247.490	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	2842.00		NIST Webbook
rinpol	2842.00		NIST Webbook
tb	907.85	K	Joback Method
tc	1152.03	K	Joback Method
tf	593.27	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.84	J/mol×K	907.85	Joback Method
cpg	674.20	J/mol×K	948.55	Joback Method
cpg	683.39	J/mol×K	989.24	Joback Method
cpg	691.44	J/mol×K	1029.94	Joback Method
cpg	698.40	J/mol×K	1070.64	Joback Method
cpg	704.32	J/mol×K	1111.34	Joback Method
cpg	709.24	J/mol×K	1152.03	Joback Method
dvisc	0.0003584	Pa×s	593.27	Joback Method

dvisc	0.0002355	Pa×s	645.70	Joback Method
dvisc	0.0001648	Pa×s	698.13	Joback Method
dvisc	0.0001213	Pa×s	750.56	Joback Method
dvisc	0.0000928	Pa×s	802.99	Joback Method
dvisc	0.0000735	Pa×s	855.42	Joback Method
dvisc	0.0000597	Pa×s	907.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393296&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
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