Glutaric acid, 2,3-dichlorophenyl 4-bromophenyl ester

Inchi: InChI=1S/C17H13BrCl2O4/c18-11-7-9-12(10-8-11)23-15(21)5-2-6-16(22)24-14-4-1-3-13(

InchiKey: HLRAOVLMAIGRPE-UHFFFAOYSA-N

Formula: C17H13BrCl2O4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 432.09

Physical Properties

Property code	Value	Unit	Source
gf	-189.19	kJ/mol	Joback Method
hf	-450.31	kJ/mol	Joback Method
hfus	45.95	kJ/mol	Joback Method
hvap	93.49	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	5.437		Crippen Method
mcvol	259.730	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinpol	3065.00		NIST Webbook
rinpol	3065.00		NIST Webbook
tb	950.26	K	Joback Method
tc	1197.71	K	Joback Method
tf	635.71	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.19	J/mol×K	950.26	Joback Method
cpg	689.15	J/mol×K	991.50	Joback Method
cpg	696.95	J/mol×K	1032.74	Joback Method
cpg	703.62	J/mol×K	1073.99	Joback Method
cpg	709.21	J/mol×K	1115.23	Joback Method
cpg	713.75	J/mol×K	1156.47	Joback Method
cpg	717.28	J/mol×K	1197.71	Joback Method
dvisc	0.0002727	Pa×s	635.71	Joback Method

dvisc	0.0001861	Pa×s	688.13	Joback Method
dvisc	0.0001341	Pa×s	740.56	Joback Method
dvisc	0.0001009	Pa×s	792.99	Joback Method
dvisc	0.0000786	Pa×s	845.41	Joback Method
dvisc	0.0000631	Pa×s	897.84	Joback Method
dvisc	0.0000518	Pa×s	950.26	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=U393297&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