Glutaric acid, 3-chlorophenyl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C18H16BrClO5/c1-23-16-10-12(19)8-9-15(16)25-18(22)7-3-6-17(21)24-14-5-2-4-13(20)11-14/h2,4-5,8-11H,3,6-7H2,1H3

InchiKey: CRSHMTBQLXOWRG-UHFFFAOYSA-N

Formula: C18H16BrClO5

SMILES: COc1cc(Br)ccc1OC(=O)CCCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 427.67

Physical Properties

Property code	Value	Unit	Source
gf	-273.84	kJ/mol	Joback Method
hf	-587.43	kJ/mol	Joback Method
hfus	45.53	kJ/mol	Joback Method
hvap	93.74	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	4.792		Crippen Method
mcvol	267.450	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	3005.00		NIST Webbook
rinpol	3005.00		NIST Webbook
tb	958.13	K	Joback Method
tc	1198.83	K	Joback Method
tf	639.29	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.70	J/mol×K	958.13	Joback Method
cpg	752.28	J/mol×K	998.25	Joback Method
cpg	760.52	J/mol×K	1038.36	Joback Method
cpg	767.42	J/mol×K	1078.48	Joback Method
cpg	773.01	J/mol×K	1118.59	Joback Method
cpg	777.29	J/mol×K	1158.71	Joback Method
cpg	780.29	J/mol×K	1198.83	Joback Method
dvisc	0.0002105	Pa×s	639.29	Joback Method

dvisc	0.0001428	Pa×s	692.43	Joback Method
dvisc	0.0001023	Pa×s	745.57	Joback Method
dvisc	0.0000767	Pa×s	798.71	Joback Method
dvisc	0.0000596	Pa×s	851.85	Joback Method
dvisc	0.0000477	Pa×s	904.99	Joback Method
dvisc	0.0000391	Pa×s	958.13	Joback Method

Sources

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=U393892&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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