Glutaric acid, 3-methylbut-2-yl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C17H23ClO5/c1-11(2)12(3)22-16(19)6-5-7-17(20)23-14-9-8-13(18)10-15(14)21

InchiKey: ISFZYCWVHUVITK-UHFFFAOYSA-N

Formula: C17H23ClO5

SMILES: COc1cc(Cl)ccc1OC(=O)CCCC(=O)OC(C)C(C)C

Mol. weight [g/mol]: 342.81

Physical Properties

Property code	Value	Unit	Source
gf	-404.24	kJ/mol	Joback Method
hf	-828.74	kJ/mol	Joback Method
hfus	36.96	kJ/mol	Joback Method
hvap	81.37	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.012		Crippen Method
mcvol	259.620	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	2341.00		NIST Webbook
rinpol	2341.00		NIST Webbook
tb	836.55	K	Joback Method
tc	1046.56	K	Joback Method
tf	499.28	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.12	J/mol×K	836.55	Joback Method
cpg	817.62	J/mol×K	1011.56	Joback Method
cpg	808.25	J/mol×K	976.56	Joback Method
cpg	797.72	J/mol×K	941.56	Joback Method
cpg	786.02	J/mol×K	906.55	Joback Method
cpg	773.15	J/mol×K	871.55	Joback Method
cpg	825.81	J/mol×K	1046.56	Joback Method
dvisc	0.0000462	Pa×s	836.55	Joback Method

dvisc	0.0000596	Pa×s	780.34	Joback Method
dvisc	0.0000799	Pa×s	724.13	Joback Method
dvisc	0.0001125	Pa×s	667.91	Joback Method
dvisc	0.0001688	Pa×s	611.70	Joback Method
dvisc	0.0002748	Pa×s	555.49	Joback Method
dvisc	0.0004995	Pa×s	499.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393903&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