Glutaric acid, 2-methylpent-3-yl 2-methyl-4-chlorophenyl ester

Inchi: InChI=1S/C18H25ClO4/c1-5-15(12(2)3)22-17(20)7-6-8-18(21)23-16-10-9-14(19)11-13(16

InchiKey: GBGWRADDMHICKG-UHFFFAOYSA-N

Formula: C18H25ClO4

SMILES: CCC(OC(=O)CCCC(=O)Oc1ccc(Cl)cc1C)C(C)C

Mol. weight [g/mol]: 340.84

Physical Properties

Property code	Value	Unit	Source
gf	-290.82	kJ/mol	Joback Method
hf	-717.16	kJ/mol	Joback Method
hfus	38.36	kJ/mol	Joback Method
hvap	81.18	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.702		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	2320.00		NIST Webbook
rinpol	2320.00		NIST Webbook
tb	837.01	K	Joback Method
tc	1046.42	K	Joback Method
tf	488.32	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.55	J/mol×K	837.01	Joback Method
cpg	803.29	J/mol×K	871.91	Joback Method
cpg	816.88	J/mol×K	906.81	Joback Method
cpg	829.36	J/mol×K	941.71	Joback Method
cpg	840.73	J/mol×K	976.62	Joback Method
cpg	851.02	J/mol×K	1011.52	Joback Method
cpg	860.23	J/mol×K	1046.42	Joback Method
dvisc	0.0006455	Pa×s	488.32	Joback Method

dvisc	0.0003418	Pa×s	546.44	Joback Method
dvisc	0.0002045	Pa×s	604.55	Joback Method
dvisc	0.0001339	Pa×s	662.66	Joback Method
dvisc	0.0000939	Pa×s	720.78	Joback Method
dvisc	0.0000694	Pa×s	778.89	Joback Method
dvisc	0.0000535	Pa×s	837.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392066&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