Glutaric acid, 4-chloro-3-methylphenyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C20H29ClO4/c1-14(12-20(3,4)5)13-24-18(22)7-6-8-19(23)25-16-9-10-17(21)15

InchiKey: ZRAYAHCJHGISPV-UHFFFAOYSA-N

Formula: C20H29ClO4

SMILES: Cc1cc(OC(=O)CCCC(=O)OCC(C)CC(C)(C)C)ccc1Cl

Mol. weight [g/mol]: 368.89

Physical Properties

Property code	Value	Unit	Source
gf	-268.70	kJ/mol	Joback Method
hf	-761.91	kJ/mol	Joback Method
hfus	39.65	kJ/mol	Joback Method
hvap	84.73	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.340		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1317.52	kPa	Joback Method
rinpol	2523.00		NIST Webbook
rinpol	2523.00		NIST Webbook
tb	879.98	K	Joback Method
tc	1092.60	K	Joback Method
tf	528.28	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.39	J/mol×K	879.98	Joback Method
cpg	920.50	J/mol×K	915.42	Joback Method
cpg	934.42	J/mol×K	950.85	Joback Method
cpg	947.21	J/mol×K	986.29	Joback Method
cpg	958.89	J/mol×K	1021.73	Joback Method
cpg	969.52	J/mol×K	1057.16	Joback Method
cpg	979.12	J/mol×K	1092.60	Joback Method
dvisc	0.0004195	Pa×s	528.28	Joback Method

dvisc	0.0002243	Pa×s	586.90	Joback Method
dvisc	0.0001344	Pa×s	645.51	Joback Method
dvisc	0.0000877	Pa×s	704.13	Joback Method
dvisc	0.0000611	Pa×s	762.75	Joback Method
dvisc	0.0000448	Pa×s	821.36	Joback Method
dvisc	0.0000343	Pa×s	879.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391538&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