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

Inchi: InChI=1S/C20H29ClO4/c1-4-6-8-16(5-2)14-24-19(22)9-7-10-20(23)25-17-11-12-18(21)15

InchiKey: JXIYSOJJFJQRPS-UHFFFAOYSA-N

Formula: C20H29ClO4

SMILES: CCCCC(CC)COC(=O)CCCC(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 368.89

Physical Properties

Property code	Value	Unit	Source
gf	-271.54	kJ/mol	Joback Method
hf	-753.16	kJ/mol	Joback Method
hfus	47.07	kJ/mol	Joback Method
hvap	86.02	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.484		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	2592.00		NIST Webbook
rinpol	2592.00		NIST Webbook
tb	883.21	K	Joback Method
tc	1090.95	K	Joback Method
tf	525.86	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.62	J/mol×K	883.21	Joback Method
cpg	919.59	J/mol×K	917.83	Joback Method
cpg	933.37	J/mol×K	952.46	Joback Method
cpg	945.98	J/mol×K	987.08	Joback Method
cpg	957.44	J/mol×K	1021.70	Joback Method
cpg	967.77	J/mol×K	1056.32	Joback Method
cpg	977.00	J/mol×K	1090.95	Joback Method
dvisc	0.0004662	Pa×s	525.86	Joback Method

dvisc	0.0002574	Pa×s	585.42	Joback Method
dvisc	0.0001586	Pa×s	644.98	Joback Method
dvisc	0.0001060	Pa×s	704.54	Joback Method
dvisc	0.0000755	Pa×s	764.09	Joback Method
dvisc	0.0000565	Pa×s	823.65	Joback Method
dvisc	0.0000439	Pa×s	883.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391473&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