Glutaric acid, (2-chlorocyclohexyl)methyl 2-ethylhexyl ester

Inchi: InChI=1S/C20H35ClO4/c1-3-5-9-16(4-2)14-24-19(22)12-8-13-20(23)25-15-17-10-6-7-11-

InchiKey: XRKZGIIEEUSVIF-UHFFFAOYSA-N

Formula: C20H35ClO4

SMILES: CCCCC(CC)COC(=O)CCCC(=O)OCC1CCCCC1Cl

Mol. weight [g/mol]: 374.94

Physical Properties

Property code	Value	Unit	Source
gf	-347.95	kJ/mol	Joback Method
hf	-932.77	kJ/mol	Joback Method
hfus	46.71	kJ/mol	Joback Method
hvap	82.54	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.257		Crippen Method
mcvol	308.920	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
rinpol	2592.00		NIST Webbook
tb	861.45	K	Joback Method
tc	1063.69	K	Joback Method
tf	477.54	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.36	J/mol×K	861.45	Joback Method
cpg	1019.41	J/mol×K	895.16	Joback Method
cpg	1036.07	J/mol×K	928.86	Joback Method
cpg	1051.35	J/mol×K	962.57	Joback Method
cpg	1065.27	J/mol×K	996.28	Joback Method
cpg	1077.86	J/mol×K	1029.99	Joback Method
cpg	1089.13	J/mol×K	1063.69	Joback Method
dvisc	0.0009325	Pa×s	477.54	Joback Method
dvisc	0.0004421	Pa×s	541.52	Joback Method

dvisc	0.0002455	Pa×s	605.51	Joback Method
dvisc	0.0001525	Pa×s	669.49	Joback Method
dvisc	0.0001029	Pa×s	733.48	Joback Method
dvisc	0.0000740	Pa×s	797.46	Joback Method
dvisc	0.0000559	Pa×s	861.45	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U405447&Units=SI

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