Glutaric acid, cyclohexylmethyl 4-chlorobenzyl ester

Inchi: InChI=1S/C19H25ClO4/c20-17-11-9-16(10-12-17)14-24-19(22)8-4-7-18(21)23-13-15-5-2

InchiKey: IDJGLQVXSWFXBI-UHFFFAOYSA-N

Formula: C19H25ClO4

SMILES: O=C(CCCC(=O)OCC1CCCCC1)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 352.85

Physical Properties

Property code	Value	Unit	Source
gf	-243.44	kJ/mol	Joback Method
hf	-661.45	kJ/mol	Joback Method
hfus	40.22	kJ/mol	Joback Method
hvap	83.95	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.677		Crippen Method
mcvol	271.070	ml/mol	McGowan Method
pc	1644.42	kPa	Joback Method
rinpol	2705.00		NIST Webbook
rinpol	2705.00		NIST Webbook
tb	875.34	K	Joback Method
tc	1099.70	K	Joback Method
tf	524.45	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.52	J/mol×K	875.34	Joback Method
cpg	903.43	J/mol×K	1062.30	Joback Method
cpg	893.65	J/mol×K	1024.91	Joback Method
cpg	882.50	J/mol×K	987.52	Joback Method
cpg	869.95	J/mol×K	950.13	Joback Method
cpg	855.97	J/mol×K	912.73	Joback Method
cpg	911.88	J/mol×K	1099.70	Joback Method
dvisc	0.0000564	Pa×s	875.34	Joback Method

dvisc	0.0000728	Pa×s	816.86	Joback Method
dvisc	0.0000977	Pa×s	758.38	Joback Method
dvisc	0.0001376	Pa×s	699.89	Joback Method
dvisc	0.0002065	Pa×s	641.41	Joback Method
dvisc	0.0003360	Pa×s	582.93	Joback Method
dvisc	0.0006096	Pa×s	524.45	Joback Method

Sources

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=U391730&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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