Glutaric acid, 4-chloro-3-methylphenyl 3,7-dimethyloctyl ester

Inchi: InChI=1S/C22H33ClO4/c1-16(2)7-5-8-17(3)13-14-26-21(24)9-6-10-22(25)27-19-11-12-20

InchiKey: ZJEPQWUZCQRSNP-UHFFFAOYSA-N

Formula: C22H33ClO4

SMILES: Cc1cc(OC(=O)CCCC(=O)OCCC(C)CCCC(C)C)ccc1Cl

Mol. weight [g/mol]: 396.95

Physical Properties

Property code	Value	Unit	Source
gf	-257.14	kJ/mol	Joback Method
hf	-799.72	kJ/mol	Joback Method
hfus	48.72	kJ/mol	Joback Method
hvap	90.09	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	6.120		Crippen Method
mcvol	324.200	ml/mol	McGowan Method
pc	1142.89	kPa	Joback Method
rinpol	2792.00		NIST Webbook
rinpol	2792.00		NIST Webbook
tb	928.53	K	Joback Method
tc	1140.93	K	Joback Method
tf	533.40	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.48	J/mol×K	928.53	Joback Method
cpg	1088.25	J/mol×K	1105.53	Joback Method
cpg	1078.04	J/mol×K	1070.13	Joback Method
cpg	1066.58	J/mol×K	1034.73	Joback Method
cpg	1053.86	J/mol×K	999.33	Joback Method
cpg	1039.83	J/mol×K	963.93	Joback Method
cpg	1097.26	J/mol×K	1140.93	Joback Method
dvisc	0.0000299	Pa×s	928.53	Joback Method

dvisc	0.0000392	Pa×s	862.67	Joback Method
dvisc	0.0000537	Pa×s	796.82	Joback Method
dvisc	0.0000780	Pa×s	730.97	Joback Method
dvisc	0.0001219	Pa×s	665.11	Joback Method
dvisc	0.0002102	Pa×s	599.26	Joback Method
dvisc	0.0004146	Pa×s	533.40	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=U391489&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