Glutaric acid, 2-(4-chlorophenyl)ethyl tetradecyl ester

Inchi: InChI=1S/C27H43ClO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-22-31-26(29)15-14-16-27(30)32-

InchiKey: KDZDSRWTVTYISQ-UHFFFAOYSA-N

Formula: C27H43ClO4

SMILES: CCCCCCCCCCCCCCOC(=O)CCCC(=O)OCCc1ccc(Cl)cc1

Mol. weight [g/mol]: 467.08

Physical Properties

Property code	Value	Unit	Source
gf	-200.53	kJ/mol	Joback Method
hf	-880.89	kJ/mol	Joback Method
hfus	69.11	kJ/mol	Joback Method
hvap	101.33	kJ/mol	Joback Method
log10ws	-8.64		Crippen Method
logp	7.840		Crippen Method
mcvol	394.650	ml/mol	McGowan Method
pc	845.54	kPa	Joback Method
rinpol	3355.00		NIST Webbook
rinpol	3355.00		NIST Webbook
tb	1038.83	K	Joback Method
tc	1276.26	K	Joback Method
tf	607.23	K	Joback Method
vc	1.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.19	J/mol×K	1038.83	Joback Method
cpg	1348.93	J/mol×K	1078.40	Joback Method
cpg	1363.95	J/mol×K	1117.97	Joback Method
cpg	1377.32	J/mol×K	1157.54	Joback Method
cpg	1389.11	J/mol×K	1197.12	Joback Method
cpg	1399.40	J/mol×K	1236.69	Joback Method
cpg	1408.26	J/mol×K	1276.26	Joback Method
dvisc	0.0002112	Pa×s	607.23	Joback Method

dvisc	0.0001099	Pa×s	679.16	Joback Method
dvisc	0.0000649	Pa×s	751.10	Joback Method
dvisc	0.0000420	Pa×s	823.03	Joback Method
dvisc	0.0000291	Pa×s	894.96	Joback Method
dvisc	0.0000213	Pa×s	966.90	Joback Method
dvisc	0.0000163	Pa×s	1038.83	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=U377310&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

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