

Glutaric acid, 2-methyl-4-chlorophenyl propyl ester

Inchi: InChI=1S/C15H19ClO4/c1-3-9-19-14(17)5-4-6-15(18)20-13-8-7-12(16)10-11(13)2/h7-8,1
InchiKey: VHHFTKZEWMGSNH-UHFFFAOYSA-N
Formula: C15H19ClO4
SMILES: CCCOC(=O)CCCC(=O)Oc1ccc(Cl)cc1C
Mol. weight [g/mol]: 298.76

Physical Properties

Property code	Value	Unit	Source
gf	-311.20	kJ/mol	Joback Method
hf	-644.68	kJ/mol	Joback Method
hfus	37.64	kJ/mol	Joback Method
hvap	75.28	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.677		Crippen Method
mcvol	225.570	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	2176.00		NIST Webbook
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tb	769.25	K	Joback Method
tc	977.26	K	Joback Method
tf	484.51	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.97	J/mol×K	769.25	Joback Method
cpg	677.58	J/mol×K	942.59	Joback Method
cpg	667.71	J/mol×K	907.92	Joback Method
cpg	656.93	J/mol×K	873.25	Joback Method
cpg	645.21	J/mol×K	838.59	Joback Method
cpg	632.56	J/mol×K	803.92	Joback Method
cpg	686.52	J/mol×K	977.26	Joback Method
dvisc	0.0000950	Pa×s	769.25	Joback Method

dvisc	0.0001183	Pa×s	721.79	Joback Method
dvisc	0.0001519	Pa×s	674.34	Joback Method
dvisc	0.0002024	Pa×s	626.88	Joback Method
dvisc	0.0002829	Pa×s	579.42	Joback Method
dvisc	0.0004197	Pa×s	531.97	Joback Method
dvisc	0.0006726	Pa×s	484.51	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=U359012&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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