Glutaric acid, 2-chlorophenyl isobutyl ester

Inchi: InChI=1S/C15H19ClO4/c1-11(2)10-19-14(17)8-5-9-15(18)20-13-7-4-3-6-12(13)16/h3-4,6
InchiKey: ASRHNDUBGQJULT-UHFFFAOYSA-N
Formula: C15H19ClO4
SMILES: CC(C)COC(=O)CCCC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]: 298.76

Physical Properties

Property code	Value	Unit	Source
gf	-304.01	kJ/mol	Joback Method
hf	-638.49	kJ/mol	Joback Method
hfus	34.51	kJ/mol	Joback Method
hvap	74.23	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.615		Crippen Method
mcvol	225.570	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook
tb	763.83	K	Joback Method
tc	974.13	K	Joback Method
tf	456.99	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.63	J/mol×K	763.83	Joback Method
cpg	634.52	J/mol×K	798.88	Joback Method
cpg	647.43	J/mol×K	833.93	Joback Method
cpg	659.36	J/mol×K	868.98	Joback Method
cpg	670.31	J/mol×K	904.03	Joback Method
cpg	680.32	J/mol×K	939.08	Joback Method
cpg	689.38	J/mol×K	974.13	Joback Method
dvisc	0.0008947	Pa×s	456.99	Joback Method

dvisc	0.0004991	Pa×s	508.13	Joback Method
dvisc	0.0003097	Pa×s	559.27	Joback Method
dvisc	0.0002082	Pa×s	610.41	Joback Method
dvisc	0.0001489	Pa×s	661.55	Joback Method
dvisc	0.0001117	Pa×s	712.69	Joback Method
dvisc	0.0000870	Pa×s	763.83	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=U358598&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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