

Glutaric acid, 3-methylbut-2-yl 2-chlorophenyl ester

Inchi:	InChI=1S/C16H21ClO4/c1-11(2)12(3)20-15(18)9-6-10-16(19)21-14-8-5-4-7-13(14)17/h4-
InchiKey:	JRFQHQPDKJFJJV-UHFFFAOYSA-N
Formula:	C16H21ClO4
SMILES:	CC(C)C(C)OC(=O)CCCC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]:	312.79

Physical Properties

Property code	Value	Unit	Source
gf	-298.03	kJ/mol	Joback Method
hf	-664.41	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	76.07	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.003		Crippen Method
mvol	239.660	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	2092.00		NIST Webbook
rinpol	2092.00		NIST Webbook
tb	786.27	K	Joback Method
tc	997.58	K	Joback Method
tf	453.26	K	Joback Method
vc	0.908	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.33	J/molxK	786.27	Joback Method
cpg	690.72	J/molxK	821.49	Joback Method
cpg	704.05	J/molxK	856.71	Joback Method
cpg	716.33	J/molxK	891.92	Joback Method
cpg	727.57	J/molxK	927.14	Joback Method
cpg	737.79	J/molxK	962.36	Joback Method
cpg	747.01	J/molxK	997.58	Joback Method
dvisc	0.0009423	Paxs	453.26	Joback Method

dvisc	0.0004823	Paxs	508.76	Joback Method
dvisc	0.0002816	Paxs	564.26	Joback Method
dvisc	0.0001811	Paxs	619.76	Joback Method
dvisc	0.0001252	Paxs	675.27	Joback Method
dvisc	0.0000916	Paxs	730.77	Joback Method
dvisc	0.0000700	Paxs	786.27	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=U391884&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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