

Glutaric acid, 3-methylbut-2-yl 2-methyl-4-chlorophenyl ester

Inchi:	InChI=1S/C17H23ClO4/c1-11(2)13(4)21-16(19)6-5-7-17(20)22-15-9-8-14(18)10-12(15)3
InchiKey:	LTZPOELVUBZTQH-UHFFFAOYSA-N
Formula:	C17H23ClO4
SMILES:	<chem>Cc1cc(Cl)ccc1OC(=O)CCCC(=O)OC(C)C(C)C</chem>
Mol. weight [g/mol]:	326.81

Physical Properties

Property code	Value	Unit	Source
gf	-299.24	kJ/mol	Joback Method
hf	-696.52	kJ/mol	Joback Method
hfus	35.77	kJ/mol	Joback Method
hvap	78.96	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.312		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2238.00		NIST Webbook
tb	814.13	K	Joback Method
tc	1024.57	K	Joback Method
tf	477.05	K	Joback Method
vc	0.965	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.48	J/molxK	814.13	Joback Method
cpg	746.01	J/molxK	849.20	Joback Method
cpg	759.44	J/molxK	884.28	Joback Method
cpg	771.80	J/molxK	919.35	Joback Method
cpg	783.08	J/molxK	954.42	Joback Method
cpg	793.30	J/molxK	989.50	Joback Method
cpg	802.47	J/molxK	1024.57	Joback Method
dvisc	0.0007140	Paxs	477.05	Joback Method

dvisc	0.0003826	Paxs	533.23	Joback Method
dvisc	0.0002309	Paxs	589.41	Joback Method
dvisc	0.0001521	Paxs	645.59	Joback Method
dvisc	0.0001072	Paxs	701.77	Joback Method
dvisc	0.0000795	Paxs	757.95	Joback Method
dvisc	0.0000615	Paxs	814.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392065&Units=SI
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

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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