

Glutaric acid, 1-cyclopentylethyl 3-chlorophenyl ester

Inchi:	InChI=1S/C18H23ClO4/c1-13(14-6-2-3-7-14)22-17(20)10-5-11-18(21)23-16-9-4-8-15(19)
InchiKey:	SKVAPNVOYCZONW-UHFFFAOYSA-N
Formula:	C18H23ClO4
SMILES:	CC(OC(=O)CCCC(=O)Oc1cccc(Cl)c1)C1CCCC1
Mol. weight [g/mol]:	338.83

Physical Properties

Property code	Value	Unit	Source
gf	-242.20	kJ/mol	Joback Method
hf	-639.93	kJ/mol	Joback Method
hfus	36.21	kJ/mol	Joback Method
hvap	81.17	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.538		Crippen Method
mvol	256.980	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	2436.00		NIST Webbook
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tb	847.75	K	Joback Method
tc	1072.16	K	Joback Method
tf	501.70	K	Joback Method
vc	0.968	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.25	J/molxK	847.75	Joback Method
cpg	842.99	J/molxK	1034.76	Joback Method
cpg	832.78	J/molxK	997.36	Joback Method
cpg	821.34	J/molxK	959.96	Joback Method
cpg	808.63	J/molxK	922.55	Joback Method
cpg	794.61	J/molxK	885.15	Joback Method
cpg	852.00	J/molxK	1072.16	Joback Method
dvisc	0.0000860	Paxs	847.75	Joback Method

dvisc	0.0001098	Paxs	790.08	Joback Method
dvisc	0.0001458	Paxs	732.40	Joback Method
dvisc	0.0002032	Paxs	674.73	Joback Method
dvisc	0.0003013	Paxs	617.05	Joback Method
dvisc	0.0004846	Paxs	559.38	Joback Method
dvisc	0.0008695	Paxs	501.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405466&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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