

Glutaric acid, cyclopentyl 3-chlorophenyl ester

Inchi: InChI=1S/C16H19ClO4/c17-12-5-3-8-14(11-12)21-16(19)10-4-9-15(18)20-13-6-1-2-7-13/
InchiKey: IOVXNILXMLJCRA-UHFFFAOYSA-N
Formula: C16H19ClO4
SMILES: O=C(CCCC(=O)OC1CCCC1)Oc1cccc(Cl)c1
Mol. weight [g/mol]: 310.77

Physical Properties

Property code	Value	Unit	Source
gf	-256.60	kJ/mol	Joback Method
hf	-593.37	kJ/mol	Joback Method
hfus	34.55	kJ/mol	Joback Method
hvap	77.10	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.901		Crippen Method
mcvol	228.800	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpola	2301.00		NIST Webbook
rinpola	2301.00		NIST Webbook
tb	802.43	K	Joback Method
tc	1028.88	K	Joback Method
tf	494.16	K	Joback Method
vc	0.862	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.13	J/molxK	802.43	Joback Method
cpg	727.62	J/molxK	991.14	Joback Method
cpg	717.53	J/molxK	953.40	Joback Method
cpg	706.27	J/molxK	915.66	Joback Method
cpg	693.80	J/molxK	877.91	Joback Method
cpg	680.10	J/molxK	840.17	Joback Method
cpg	736.57	J/molxK	1028.88	Joback Method
dvisc	0.0001224	Paxs	802.43	Joback Method

dvisc	0.0001530	Paxs	751.05	Joback Method
dvisc	0.0001976	Paxs	699.67	Joback Method
dvisc	0.0002658	Paxs	648.29	Joback Method
dvisc	0.0003763	Paxs	596.92	Joback Method
dvisc	0.0005687	Paxs	545.54	Joback Method
dvisc	0.0009367	Paxs	494.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405397&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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