

Glutaric acid, cyclohexylmethyl 2-methyl-4-chlorophenyl ester

Inchi:	InChI=1S/C19H25ClO4/c1-14-12-16(20)10-11-17(14)24-19(22)9-5-8-18(21)23-13-15-6-3
InchiKey:	NQTTVJBYPWCWEI-UHFFFAOYSA-N
Formula:	C19H25ClO4
SMILES:	<chem>Cc1cc(Cl)ccc1OC(=O)CCCC(=O)OCC1CCCCC1</chem>
Mol. weight [g/mol]:	352.85

Physical Properties

Property code	Value	Unit	Source
gf	-253.07	kJ/mol	Joback Method
hf	-672.92	kJ/mol	Joback Method
hfus	39.83	kJ/mol	Joback Method
hvap	84.61	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.848		Crippen Method
mcvol	271.070	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	2672.00		NIST Webbook
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tb	880.32	K	Joback Method
tc	1105.43	K	Joback Method
tf	536.97	K	Joback Method
vc	1.022	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.57	J/molxK	880.32	Joback Method
cpg	854.90	J/molxK	917.84	Joback Method
cpg	868.74	J/molxK	955.36	Joback Method
cpg	881.14	J/molxK	992.88	Joback Method
cpg	892.11	J/molxK	1030.40	Joback Method
cpg	901.69	J/molxK	1067.91	Joback Method
cpg	909.89	J/molxK	1105.43	Joback Method
dvisc	0.0005300	Paxs	536.97	Joback Method

dvisc	0.0003060	Paxs	594.20	Joback Method
dvisc	0.0001946	Paxs	651.42	Joback Method
dvisc	0.0001331	Paxs	708.64	Joback Method
dvisc	0.0000964	Paxs	765.87	Joback Method
dvisc	0.0000730	Paxs	823.10	Joback Method
dvisc	0.0000573	Paxs	880.32	Joback Method

Sources

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=U392073&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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