

Glutaric acid, oct-1-en-3-yl 3-chlorophenyl ester

Inchi:	InChI=1S/C19H25ClO4/c1-3-5-6-10-16(4-2)23-18(21)12-8-13-19(22)24-17-11-7-9-15(20)
InchiKey:	PPPPJTBXQPOUGS-UHFFFAOYSA-N
Formula:	C19H25ClO4
SMILES:	<chem>C=CC(CCCCC)OC(=O)CCCC(=O)Oc1cccc(Cl)c1</chem>
Mol. weight [g/mol]:	352.85

Physical Properties

Property code	Value	Unit	Source
gf	-182.49	kJ/mol	Joback Method
hf	-595.62	kJ/mol	Joback Method
hfus	43.59	kJ/mol	Joback Method
hvap	82.47	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.094		Crippen Method
mcvol	277.630	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpola	2411.00		NIST Webbook
tb	852.03	K	Joback Method
tc	1059.99	K	Joback Method
tf	500.31	K	Joback Method
vc	1.063	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.41	J/molxK	852.03	Joback Method
cpg	880.65	J/molxK	1025.33	Joback Method
cpg	870.49	J/molxK	990.67	Joback Method
cpg	859.32	J/molxK	956.01	Joback Method
cpg	847.10	J/molxK	921.35	Joback Method
cpg	833.80	J/molxK	886.69	Joback Method
cpg	889.82	J/molxK	1059.99	Joback Method
dvisc	0.0000535	Paxs	852.03	Joback Method
dvisc	0.0000692	Paxs	793.41	Joback Method

dvisc	0.0000932	Paxs	734.79	Joback Method
dvisc	0.0001322	Paxs	676.17	Joback Method
dvisc	0.0002004	Paxs	617.55	Joback Method
dvisc	0.0003314	Paxs	558.93	Joback Method
dvisc	0.0006166	Paxs	500.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405354&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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