

Glutaric acid, hex-2-en-1-yl 3-chlorophenyl ester

Inchi:	InChI=1S/C17H21ClO4/c1-2-3-4-5-12-21-16(19)10-7-11-17(20)22-15-9-6-8-14(18)13-15
InchiKey:	XAJIUAJNVQFKMX-SNAWJCMRSA-N
Formula:	C17H21ClO4
SMILES:	CCCC=CCOC(=O)CCCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	324.80

Physical Properties

Property code	Value	Unit	Source
gf	-204.51	kJ/mol	Joback Method
hf	-557.27	kJ/mol	Joback Method
hfus	43.41	kJ/mol	Joback Method
hvap	79.03	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.315		Crippen Method
mvol	249.450	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2314.00		NIST Webbook
rinpol	2314.00		NIST Webbook
tb	814.19	K	Joback Method
tc	1024.15	K	Joback Method
tf	489.45	K	Joback Method
vc	0.957	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.27	J/molxK	814.19	Joback Method
cpg	764.61	J/molxK	989.16	Joback Method
cpg	754.59	J/molxK	954.16	Joback Method
cpg	743.68	J/molxK	919.17	Joback Method
cpg	731.84	J/molxK	884.18	Joback Method
cpg	719.05	J/molxK	849.18	Joback Method
cpg	773.76	J/molxK	1024.15	Joback Method
dvisc	0.0000629	Paxs	814.19	Joback Method

dvisc	0.0000802	Paxs	760.07	Joback Method
dvisc	0.0001061	Paxs	705.94	Joback Method
dvisc	0.0001471	Paxs	651.82	Joback Method
dvisc	0.0002163	Paxs	597.70	Joback Method
dvisc	0.0003435	Paxs	543.57	Joback Method
dvisc	0.0006045	Paxs	489.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405335&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

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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