Glutaric acid, hex-4-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: HWKPURINCFHHTK-NSCUHMNNSA-N

Formula: C17H21ClO4

SMILES: CC=CCCCOC(=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
mcvol	249.450	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook
tb	814.19	K	Joback Method
tc	1024.15	K	Joback Method
tf	489.45	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000802	Pa×s	760.07	Joback Method
dvisc	0.0001061	Pa×s	705.94	Joback Method
dvisc	0.0001471	Pa×s	651.82	Joback Method
dvisc	0.0002163	Pa×s	597.70	Joback Method
dvisc	0.0003435	Pa×s	543.57	Joback Method
dvisc	0.0006045	Pa×s	489.45	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=U405305&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