

Glutaric acid, dec-2-yl 2-methyl-4-chlorophenyl ester

Inchi:	InChI=1S/C22H33ClO4/c1-4-5-6-7-8-9-11-18(3)26-21(24)12-10-13-22(25)27-20-15-14-19
InchiKey:	FXSJIXPFQXQDJQ-UHFFFAOYSA-N
Formula:	C22H33ClO4
SMILES:	CCCCCCCC(C)OC(=O)CCCC(=O)Oc1ccc(Cl)cc1C
Mol. weight [g/mol]:	396.95

Physical Properties

Property code	Value	Unit	Source
gf	-254.70	kJ/mol	Joback Method
hf	-794.44	kJ/mol	Joback Method
hfus	52.25	kJ/mol	Joback Method
hvap	90.48	kJ/mol	Joback Method
log10ws	-7.36		Crippen Method
logp	6.406		Crippen Method
mvol	324.200	ml/mol	McGowan Method
pc	1136.73	kPa	Joback Method
rinpol	2745.00		NIST Webbook
rinpol	2745.00		NIST Webbook
tb	928.97	K	Joback Method
tc	1140.43	K	Joback Method
tf	548.40	K	Joback Method
vc	1.250	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.02	J/molxK	928.97	Joback Method
cpg	1039.35	J/molxK	964.21	Joback Method
cpg	1053.36	J/molxK	999.46	Joback Method
cpg	1066.11	J/molxK	1034.70	Joback Method
cpg	1077.60	J/molxK	1069.94	Joback Method
cpg	1087.88	J/molxK	1105.19	Joback Method
cpg	1096.97	J/molxK	1140.43	Joback Method
dvisc	0.0003736	Paxs	548.40	Joback Method

dvisc	0.0002018	Paxs	611.83	Joback Method
dvisc	0.0001224	Paxs	675.26	Joback Method
dvisc	0.0000809	Paxs	738.68	Joback Method
dvisc	0.0000570	Paxs	802.11	Joback Method
dvisc	0.0000424	Paxs	865.54	Joback Method
dvisc	0.0000328	Paxs	928.97	Joback Method

Sources

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=U392076&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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