

Glutaric acid, dodec-2-en-1-yl 8-chlorooctyl ester

Inchi:	InChI=1S/C25H45ClO4/c1-2-3-4-5-6-7-8-10-13-16-22-29-24(27)19-18-20-25(28)30-23-17
InchiKey:	BRXYOVWXWCIEV-DTQAZKPQSA-N
Formula:	C25H45ClO4
SMILES:	CCCCCCCCC=CCOC(=O)CCCC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	445.07

Physical Properties

Property code	Value	Unit	Source
gf	-239.93	kJ/mol	Joback Method
hf	-947.45	kJ/mol	Joback Method
hfus	70.48	kJ/mol	Joback Method
hvap	93.90	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	7.519		Crippen Method
mvol	385.930	ml/mol	McGowan Method
pc	811.22	kPa	Joback Method
rinpol	3173.00		NIST Webbook
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tb	965.57	K	Joback Method
tc	1186.60	K	Joback Method
tf	540.67	K	Joback Method
vc	1.512	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1283.75	J/molxK	965.57	Joback Method
cpg	1303.05	J/molxK	1002.41	Joback Method
cpg	1320.89	J/molxK	1039.25	Joback Method
cpg	1337.34	J/molxK	1076.09	Joback Method
cpg	1352.48	J/molxK	1112.93	Joback Method
cpg	1366.35	J/molxK	1149.76	Joback Method
cpg	1379.04	J/molxK	1186.60	Joback Method
dvisc	0.0003323	Paxs	540.67	Joback Method

dvisc	0.0001554	Paxs	611.49	Joback Method
dvisc	0.0000851	Paxs	682.30	Joback Method
dvisc	0.0000522	Paxs	753.12	Joback Method
dvisc	0.0000348	Paxs	823.94	Joback Method
dvisc	0.0000247	Paxs	894.75	Joback Method
dvisc	0.0000185	Paxs	965.57	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393467&Units=SI

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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