

Glutaric acid, 3-methylbut-2-en-1-yl 10-chlorodecyl ester

Inchi: InChI=1S/C20H35ClO4/c1-18(2)14-17-25-20(23)13-11-12-19(22)24-16-10-8-6-4-3-5-7-9
InchiKey: HZGBJVUWQMTDJW-UHFFFAOYSA-N
Formula: C20H35ClO4
SMILES: CC(C)=CCOC(=O)CCCC(=O)OCCCCCCCCCCCCI
Mol. weight [g/mol]: 374.94

Physical Properties

Property code	Value	Unit	Source
gf	-290.58	kJ/mol	Joback Method
hf	-854.04	kJ/mol	Joback Method
hfus	56.22	kJ/mol	Joback Method
hvap	82.85	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	5.569		Crippen Method
mcvol	315.480	ml/mol	McGowan Method
pc	1092.10	kPa	Joback Method
rinpol	2675.00		NIST Webbook
rinpol	2675.00		NIST Webbook
tb	851.05	K	Joback Method
tc	1044.51	K	Joback Method
tf	470.36	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.13	J/mol×K	851.05	Joback Method
cpg	990.98	J/mol×K	883.29	Joback Method
cpg	1006.80	J/mol×K	915.54	Joback Method
cpg	1021.63	J/mol×K	947.78	Joback Method
cpg	1035.49	J/mol×K	980.03	Joback Method
cpg	1048.42	J/mol×K	1012.27	Joback Method
cpg	1060.44	J/mol×K	1044.51	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U392456&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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