

Glutaric acid, 2-methylpent-3-yl 10-chlorodecyl ester

Inchi:	InChI=1S/C21H39ClO4/c1-4-19(18(2)3)26-21(24)15-13-14-20(23)25-17-12-10-8-6-5-7-9
InchiKey:	LVSFIDVSKSCXQA-UHFFFAOYSA-N
Formula:	C21H39ClO4
SMILES:	CCC(OC(=O)CCCC(=O)OCCCCCCCCCCCCI)C(C)C
Mol. weight [g/mol]:	390.99

Physical Properties

Property code	Value	Unit	Source
gf	-358.71	kJ/mol	Joback Method
hf	-992.67	kJ/mol	Joback Method
hfus	52.87	kJ/mol	Joback Method
hvap	84.26	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	6.037		Crippen Method
mcvol	333.870	ml/mol	McGowan Method
pc	999.54	kPa	Joback Method
rinpol	2647.00		NIST Webbook
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tb	869.01	K	Joback Method
tc	1064.58	K	Joback Method
tf	470.67	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.75	J/molxK	869.01	Joback Method
cpg	1140.03	J/molxK	1031.99	Joback Method
cpg	1126.87	J/molxK	999.39	Joback Method
cpg	1112.59	J/molxK	966.80	Joback Method
cpg	1097.16	J/molxK	934.20	Joback Method
cpg	1080.55	J/molxK	901.61	Joback Method
cpg	1152.08	J/molxK	1064.58	Joback Method
dvisc	0.0000328	Paxs	869.01	Joback Method

dvisc	0.0000448	Paxs	802.62	Joback Method
dvisc	0.0000648	Paxs	736.23	Joback Method
dvisc	0.0001006	Paxs	669.84	Joback Method
dvisc	0.0001721	Paxs	603.45	Joback Method
dvisc	0.0003364	Paxs	537.06	Joback Method
dvisc	0.0007944	Paxs	470.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392455&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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