

Glutaric acid, 10-chlorodecyl dodecyl ester

Inchi: InChI=1S/C27H51ClO4/c1-2-3-4-5-6-7-9-12-15-18-24-31-26(29)21-20-22-27(30)32-25-19
InchiKey: PGAJZLBKBFPEW-UHFFFAOYSA-N
Formula: C27H51ClO4
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)OCCCCCCCCCCI
Mol. weight [g/mol]: 475.14

Physical Properties

Property code	Value	Unit	Source
gf	-303.31	kJ/mol	Joback Method
hf	-1105.95	kJ/mol	Joback Method
hfus	75.46	kJ/mol	Joback Method
hvap	98.39	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	8.524		Crippen Method
mcvol	418.410	ml/mol	McGowan Method
pc	709.22	kPa	Joback Method
rinqol	3457.00		NIST Webbook
tb	1007.17	K	Joback Method
tc	1250.03	K	Joback Method
tf	568.29	K	Joback Method
vc	1.645	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1439.54	J/molxK	1007.17	Joback Method
cpg	1460.65	J/molxK	1047.65	Joback Method
cpg	1479.77	J/molxK	1088.12	Joback Method
cpg	1496.99	J/molxK	1128.60	Joback Method
cpg	1512.38	J/molxK	1169.08	Joback Method
cpg	1526.02	J/molxK	1209.55	Joback Method
cpg	1537.98	J/molxK	1250.03	Joback Method
dvisc	0.0002741	Paxs	568.29	Joback Method
dvisc	0.0001289	Paxs	641.44	Joback Method

dvisc	0.0000707	Paxs	714.58	Joback Method
dvisc	0.0000434	Paxs	787.73	Joback Method
dvisc	0.0000289	Paxs	860.88	Joback Method
dvisc	0.0000205	Paxs	934.02	Joback Method
dvisc	0.0000153	Paxs	1007.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359405&Units=SI
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

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
mccvol:	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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