

Glutaric acid, dodec-2-en-1-yl 10-chlorodecyl ester

Inchi:	InChI=1S/C27H49ClO4/c1-2-3-4-5-6-7-9-12-15-18-24-31-26(29)21-20-22-27(30)32-25-19
InchiKey:	LHOKIKOMNFZRFY-OBGWFSINSA-N
Formula:	C27H49ClO4
SMILES:	CCCCCCCCC=CCOC(=O)CCCC(=O)OCCCCCCCCCCCCI
Mol. weight [g/mol]:	473.13

Physical Properties

Property code	Value	Unit	Source
gf	-223.09	kJ/mol	Joback Method
hf	-988.73	kJ/mol	Joback Method
hfus	75.66	kJ/mol	Joback Method
hvap	98.35	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	8.300		Crippen Method
mcvol	414.110	ml/mol	McGowan Method
pc	729.28	kPa	Joback Method
rinpol	3363.00		NIST Webbook
rinpol	3363.00		NIST Webbook
tb	1011.33	K	Joback Method
tc	1251.49	K	Joback Method
tf	563.21	K	Joback Method
vc	1.625	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1411.17	J/molxK	1011.33	Joback Method
cpg	1431.78	J/molxK	1051.36	Joback Method
cpg	1450.67	J/molxK	1091.38	Joback Method
cpg	1467.94	J/molxK	1131.41	Joback Method
cpg	1483.67	J/molxK	1171.44	Joback Method
cpg	1497.95	J/molxK	1211.46	Joback Method
cpg	1510.89	J/molxK	1251.49	Joback Method
dvisc	0.0002549	Paxs	563.21	Joback Method

dvisc	0.0001172	Paxs	637.90	Joback Method
dvisc	0.0000634	Paxs	712.58	Joback Method
dvisc	0.0000386	Paxs	787.27	Joback Method
dvisc	0.0000256	Paxs	861.96	Joback Method
dvisc	0.0000181	Paxs	936.64	Joback Method
dvisc	0.0000135	Paxs	1011.33	Joback Method

Sources

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=U392478&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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