

Glutaric acid, dodec-9-ynyl nonyl ester

Inchi:	InChI=1S/C26H46O4/c1-3-5-7-9-11-12-13-15-17-19-24-30-26(28)22-20-21-25(27)29-23-
InchiKey:	SOXAHEFYHASJRM-UHFFFAOYSA-N
Formula:	C26H46O4
SMILES:	CCC#CCCCCCCCCOC(=O)CCCC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	422.64

Physical Properties

Property code	Value	Unit	Source
gf	-97.00	kJ/mol	Joback Method
hf	-797.27	kJ/mol	Joback Method
hfus	71.79	kJ/mol	Joback Method
hvap	93.93	kJ/mol	Joback Method
log10ws	-8.23		Crippen Method
logp	7.138		Crippen Method
mvol	383.480	ml/mol	McGowan Method
pc	834.35	kPa	Joback Method
rmpol	3063.00		NIST Webbook
rmpol	3063.00		NIST Webbook
tb	955.86	K	Joback Method
tc	1172.24	K	Joback Method
tf	633.20	K	Joback Method
vc	1.502	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1290.85	J/molxK	955.86	Joback Method
cpg	1310.44	J/molxK	991.92	Joback Method
cpg	1328.48	J/molxK	1027.99	Joback Method
cpg	1345.02	J/molxK	1064.05	Joback Method
cpg	1360.10	J/molxK	1100.11	Joback Method
cpg	1373.76	J/molxK	1136.17	Joback Method
cpg	1386.04	J/molxK	1172.24	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359792&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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