

Nonanoic acid, eicosyl ester

Inchi: InChI=1S/C29H58O2/c1-3-5-7-9-11-12-13-14-15-16-17-18-19-20-21-22-24-26-28-31-29(23,25,27,29)
InchiKey: YGVAMBJJMRNOGF-UHFFFAOYSA-N
Formula: C29H58O2
SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCC
Mol. weight [g/mol]: 438.77

Physical Properties

Property code	Value	Unit	Source
gf	-40.62	kJ/mol	Joback Method
hf	-886.69	kJ/mol	Joback Method
hfus	73.65	kJ/mol	Joback Method
hvap	89.30	kJ/mol	Joback Method
log10ws	-10.82		Crippen Method
logp	10.322		Crippen Method
mvol	426.910	ml/mol	McGowan Method
pc	638.98	kPa	Joback Method
rinpol	3079.00		NIST Webbook
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tb	939.21	K	Joback Method
tc	1161.87	K	Joback Method
tf	488.75	K	Joback Method
vc	1.683	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1482.38	J/molxK	939.21	Joback Method
cpg	1507.73	J/molxK	976.32	Joback Method
cpg	1531.33	J/molxK	1013.43	Joback Method
cpg	1553.27	J/molxK	1050.54	Joback Method
cpg	1573.64	J/molxK	1087.65	Joback Method
cpg	1592.51	J/molxK	1124.76	Joback Method
cpg	1609.96	J/molxK	1161.87	Joback Method
dvisc	0.0005585	Paxs	488.75	Joback Method

dvisc	0.0002206	Paxs	563.83	Joback Method
dvisc	0.0001084	Paxs	638.90	Joback Method
dvisc	0.0000618	Paxs	713.98	Joback Method
dvisc	0.0000393	Paxs	789.06	Joback Method
dvisc	0.0000270	Paxs	864.13	Joback Method
dvisc	0.0000197	Paxs	939.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340287&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

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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