

Adipic acid, eicosyl pent-4-enyl ester

Inchi: InChI=1S/C31H58O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-29-35-31(3)
InchiKey: QCHFTUDVGAHNJF-UHFFFAOYSA-N
Formula: C31H58O4
SMILES: C=CCCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 494.79

Physical Properties

Property code	Value	Unit	Source
gf	-169.86	kJ/mol	Joback Method
hf	-1047.34	kJ/mol	Joback Method
hfus	80.34	kJ/mol	Joback Method
hvap	102.24	kJ/mol	Joback Method
log10ws	-10.38		Crippen Method
logp	9.641		Crippen Method
mcvol	458.230	ml/mol	McGowan Method
pc	606.66	kPa	Joback Method
rinqol	3433.00		NIST Webbook
tb	1057.94	K	Joback Method
tc	1335.41	K	Joback Method
tf	581.69	K	Joback Method
vc	1.800	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1639.81	J/molxK	1057.94	Joback Method
cpg	1738.03	J/molxK	1289.17	Joback Method
cpg	1722.98	J/molxK	1242.92	Joback Method
cpg	1705.79	J/molxK	1196.68	Joback Method
cpg	1686.29	J/molxK	1150.43	Joback Method
cpg	1664.34	J/molxK	1104.19	Joback Method
cpg	1751.06	J/molxK	1335.41	Joback Method
dvisc	0.0000106	Paxs	1057.94	Joback Method
dvisc	0.0000143	Paxs	978.57	Joback Method

dvisc	0.0000203	Paxs	899.19	Joback Method
dvisc	0.0000309	Paxs	819.82	Joback Method
dvisc	0.0000514	Paxs	740.44	Joback Method
dvisc	0.0000968	Paxs	661.07	Joback Method
dvisc	0.0002165	Paxs	581.69	Joback Method

Sources

Crippen Method:	https://www.chemeo.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=U353808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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