

Pimelic acid, hexyl octadecyl ester

Inchi:	InChI=1S/C31H60O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-20-25-29-35-31(33)27-
InchiKey:	KDQNBFBHJYNDMHH-UHFFFAOYSA-N
Formula:	C31H60O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCC
Mol. weight [g/mol]:	496.81

Physical Properties

Property code	Value	Unit	Source
gf	-257.70	kJ/mol	Joback Method
hf	-1172.77	kJ/mol	Joback Method
hfus	81.62	kJ/mol	Joback Method
hvap	102.91	kJ/mol	Joback Method
log10ws	-10.52		Crippen Method
logp	9.865		Crippen Method
mvol	462.530	ml/mol	McGowan Method
pc	594.30	kPa	Joback Method
rinpol	2883.00		NIST Webbook
rinpol	2883.00		NIST Webbook
tb	1061.26	K	Joback Method
tc	1344.42	K	Joback Method
tf	583.45	K	Joback Method
vc	1.819	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1670.89	J/molxK	1061.26	Joback Method
cpg	1696.10	J/molxK	1108.45	Joback Method
cpg	1718.46	J/molxK	1155.65	Joback Method
cpg	1738.13	J/molxK	1202.84	Joback Method
cpg	1755.25	J/molxK	1250.03	Joback Method
cpg	1769.95	J/molxK	1297.22	Joback Method
cpg	1782.40	J/molxK	1344.42	Joback Method
dvisc	0.0002077	Paxs	583.45	Joback Method

dvisc	0.0000918	Paxs	663.08	Joback Method
dvisc	0.0000484	Paxs	742.72	Joback Method
dvisc	0.0000288	Paxs	822.36	Joback Method
dvisc	0.0000188	Paxs	901.99	Joback Method
dvisc	0.0000132	Paxs	981.62	Joback Method
dvisc	0.0000097	Paxs	1061.26	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=U406448&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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