

Adipic acid, 2,4-dimethylpent-3-yl eicosyl ester

Inchi:	InChI=1S/C33H64O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-28-36-31(
InchiKey:	PCXIKGWOZBSKFY-UHFFFAOYSA-N
Formula:	C33H64O4
SMILES:	CCCCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	524.86

Physical Properties

Property code	Value	Unit	Source
gf	-248.18	kJ/mol	Joback Method
hf	-1229.89	kJ/mol	Joback Method
hfus	76.23	kJ/mol	Joback Method
hvap	106.20	kJ/mol	Joback Method
log10ws	-10.99		Crippen Method
logp	10.356		Crippen Method
mcvol	490.710	ml/mol	McGowan Method
pc	548.46	kPa	Joback Method
rinsol	3499.00		NIST Webbook
tb	1105.70	K	Joback Method
tc	1410.58	K	Joback Method
tf	560.99	K	Joback Method
vc	1.913	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1802.96	J/molxK	1105.70	Joback Method
cpg	1828.39	J/molxK	1156.51	Joback Method
cpg	1850.50	J/molxK	1207.33	Joback Method
cpg	1869.46	J/molxK	1258.14	Joback Method
cpg	1885.48	J/molxK	1308.95	Joback Method
cpg	1898.77	J/molxK	1359.76	Joback Method
cpg	1909.51	J/molxK	1410.58	Joback Method
dvisc	0.0002217	Paxs	560.99	Joback Method
dvisc	0.0000768	Paxs	651.77	Joback Method

dvisc	0.0000345	Paxs	742.56	Joback Method
dvisc	0.0000184	Paxs	833.35	Joback Method
dvisc	0.0000112	Paxs	924.13	Joback Method
dvisc	0.0000074	Paxs	1014.92	Joback Method
dvisc	0.0000052	Paxs	1105.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353536&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

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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