

Adipic acid, octadecyl pent-4-en-2-yl ester

Inchi:	InChI=1S/C29H54O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-26-32-28(30)24-2
InchiKey:	XROQBMOJVBWIML-UHFFFAOYSA-N
Formula:	C29H54O4
SMILES:	C=CCC(C)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	466.74

Physical Properties

Property code	Value	Unit	Source
gf	-189.14	kJ/mol	Joback Method
hf	-1011.34	kJ/mol	Joback Method
hfus	71.64	kJ/mol	Joback Method
hvap	97.40	kJ/mol	Joback Method
log10ws	-9.65		Crippen Method
logp	8.859		Crippen Method
mcvol	430.050	ml/mol	McGowan Method
pc	671.16	kPa	Joback Method
rinsol	3155.00		NIST Webbook
tb	1011.74	K	Joback Method
tc	1257.87	K	Joback Method
tf	544.15	K	Joback Method
vc	1.683	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1509.38	J/molxK	1011.74	Joback Method
cpg	1602.28	J/molxK	1216.85	Joback Method
cpg	1587.48	J/molxK	1175.83	Joback Method
cpg	1570.87	J/molxK	1134.80	Joback Method
cpg	1552.39	J/molxK	1093.78	Joback Method
cpg	1531.92	J/molxK	1052.76	Joback Method
cpg	1615.38	J/molxK	1257.87	Joback Method
dvisc	0.0000133	Paxs	1011.74	Joback Method
dvisc	0.0000181	Paxs	933.81	Joback Method

dvisc	0.0000260	Paxs	855.88	Joback Method
dvisc	0.0000404	Paxs	777.94	Joback Method
dvisc	0.0000690	Paxs	700.01	Joback Method
dvisc	0.0001351	Paxs	622.08	Joback Method
dvisc	0.0003203	Paxs	544.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354133&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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