

Tetradec-9-enoic acid docosyl ester, Z

Inchi:	InChI=1S/C36H70O2/c1-3-5-7-9-11-13-15-16-17-18-19-20-21-22-23-25-27-29-31-33-35-
InchiKey:	WPTDDMDBQMXJJJ-BENRWUELSA-N
Formula:	C36H70O2
SMILES:	CCCC=CCCCCCCC(=O)OCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	534.94

Physical Properties

Property code	Value	Unit	Source
gf	98.54	kJ/mol	Joback Method
hf	-913.95	kJ/mol	Joback Method
hfus	91.99	kJ/mol	Joback Method
hvap	104.84	kJ/mol	Joback Method
log10ws	-13.61		Crippen Method
logp	12.829		Crippen Method
mvol	521.240	ml/mol	McGowan Method
pc	477.56	kPa	Joback Method
rinpol	3743.66		NIST Webbook
rinpol	3743.66		NIST Webbook
tb	1103.53	K	Joback Method
tc	1429.86	K	Joback Method
tf	562.56	K	Joback Method
vc	2.055	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1927.12	J/molxK	1103.53	Joback Method
cpg	1960.79	J/molxK	1157.92	Joback Method
cpg	1991.51	J/molxK	1212.31	Joback Method
cpg	2019.68	J/molxK	1266.69	Joback Method
cpg	2045.69	J/molxK	1321.08	Joback Method
cpg	2069.92	J/molxK	1375.47	Joback Method
cpg	2092.76	J/molxK	1429.86	Joback Method
dvisc	0.0001922	Paxs	562.56	Joback Method

dvisc	0.0000712	Paxs	652.72	Joback Method
dvisc	0.0000336	Paxs	742.88	Joback Method
dvisc	0.0000186	Paxs	833.04	Joback Method
dvisc	0.0000116	Paxs	923.21	Joback Method
dvisc	0.0000078	Paxs	1013.37	Joback Method
dvisc	0.0000057	Paxs	1103.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R437339&Units=SI

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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