

1-Docosanol, acetate

Other names:	Docosyl acetate n-Docosyl acetate Acetic acid, docosyl ester Behenyl acetate Docosanol acetate Docosanyl acetate
Inchi:	InChI=1S/C24H48O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-26-2
InchiKey:	AWYRDXDPCQRJHE-UHFFFAOYSA-N
Formula:	C24H48O2
SMILES:	CCCCCCCCCCCCCCCCCCCCOCC(=O)
Mol. weight [g/mol]:	368.64
CAS:	822-26-4

Physical Properties

Property code	Value	Unit	Source
gf	-82.72	kJ/mol	Joback Method
hf	-783.49	kJ/mol	Joback Method
hfus	60.70	kJ/mol	Joback Method
hvap	78.17	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	8.371		Crippen Method
mcvol	356.460	ml/mol	McGowan Method
pc	827.64	kPa	Joback Method
rinpol	2611.00		NIST Webbook
rinpol	2611.30		NIST Webbook
rinpol	2611.00		NIST Webbook
rinpol	2613.00		NIST Webbook
rinpol	2617.00		NIST Webbook
rinpol	2594.00		NIST Webbook
rinpol	2604.00		NIST Webbook
rinpol	2611.00		NIST Webbook
rinpol	2609.00		NIST Webbook
tb	824.81	K	Joback Method
tc	1009.81	K	Joback Method
tf	432.40	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.81	J/molxK	824.81	Joback Method
cpg	1178.47	J/molxK	855.64	Joback Method
cpg	1198.97	J/molxK	886.48	Joback Method
cpg	1218.34	J/molxK	917.31	Joback Method
cpg	1236.63	J/molxK	948.14	Joback Method
cpg	1253.86	J/molxK	978.97	Joback Method
cpg	1270.08	J/molxK	1009.81	Joback Method
dvisc	0.0010603	Paxs	432.40	Joback Method
dvisc	0.0004342	Paxs	497.80	Joback Method
dvisc	0.0002188	Paxs	563.20	Joback Method
dvisc	0.0001271	Paxs	628.61	Joback Method
dvisc	0.0000818	Paxs	694.01	Joback Method
dvisc	0.0000568	Paxs	759.41	Joback Method
dvisc	0.0000418	Paxs	824.81	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=C822264&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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