

Eicosanyl acetate

Other names:	1-Eicosanol acetate Eicosyl acetate eicosyl ethanoate
Inchi:	InChI=1S/C22H44O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-22(2)23
InchiKey:	JUCOQIYAKWHGSZ-UHFFFAOYSA-N
Formula:	C22H44O2
SMILES:	CCCCCCCCCCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]:	340.58
CAS:	822-24-2

Physical Properties

Property code	Value	Unit	Source
gf	-99.56	kJ/mol	Joback Method
hf	-742.21	kJ/mol	Joback Method
hfus	55.52	kJ/mol	Joback Method
hvap	73.72	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.591		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	927.24	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	2393.00		NIST Webbook
rinpol	2409.10		NIST Webbook
rinpol	2413.00		NIST Webbook
rinpol	2393.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2409.10		NIST Webbook
tb	779.05	K	Joback Method
tc	955.69	K	Joback Method
tf	409.86	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.01	J/mol×K	779.05	Joback Method
cpg	1051.60	J/mol×K	808.49	Joback Method
cpg	1071.17	J/mol×K	837.93	Joback Method
cpg	1089.74	J/mol×K	867.37	Joback Method
cpg	1107.35	J/mol×K	896.81	Joback Method
cpg	1124.02	J/mol×K	926.25	Joback Method
cpg	1139.78	J/mol×K	955.69	Joback Method
dvisc	0.0013386	Paxs	409.86	Joback Method
dvisc	0.0005575	Paxs	471.39	Joback Method
dvisc	0.0002843	Paxs	532.92	Joback Method
dvisc	0.0001666	Paxs	594.45	Joback Method
dvisc	0.0001080	Paxs	655.99	Joback Method
dvisc	0.0000754	Paxs	717.52	Joback Method
dvisc	0.0000557	Paxs	779.05	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	3.04923e+01
Coeff. B	-1.29537e+04
Coeff. C	-1.48858e+02
Temperature range (K), min.	577.72
Temperature range (K), max.	663.28

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=C822242&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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