1-Docosanol, propanoate

Other names: Docosanyl propionate
Inchi: InChI=1S/C25H50O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-27
InchiKey: INLQPAGXYNKUDT-UHFFFAOYSA-N
Formula: C25H50O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCOC(=O)CC
Mol. weight [g/mol]: 382.66
CAS: 55334-75-3

Physical Properties

Property code	Value	Unit	Source
gf	-74.30	kJ/mol	Joback Method
hf	-804.13	kJ/mol	Joback Method
hfus	63.29	kJ/mol	Joback Method
hvap	80.40	kJ/mol	Joback Method
log10ws	-9.15		Crippen Method
logp	8.762		Crippen Method
mcvol	370.550	ml/mol	McGowan Method
pc	783.75	kPa	Joback Method
rinpol	2699.00		NIST Webbook
rinpol	2699.00		NIST Webbook
tb	847.69	K	Joback Method
tc	1038.15	K	Joback Method
tf	443.67	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.77	J/mol×K	847.69	Joback Method
cpg	1243.05	J/mol×K	879.43	Joback Method
cpg	1264.07	J/mol×K	911.18	Joback Method
cpg	1283.89	J/mol×K	942.92	Joback Method
cpg	1302.54	J/mol×K	974.66	Joback Method
cpg	1320.07	J/mol×K	1006.41	Joback Method

cpg	1336.53	J/mol×K	1038.15	Joback Method
dvisc	0.0009384	Pa×s	443.67	Joback Method
dvisc	0.0003813	Pa×s	511.01	Joback Method
dvisc	0.0001910	Pa×s	578.34	Joback Method
dvisc	0.0001106	Pa×s	645.68	Joback Method
dvisc	0.0000710	Pa×s	713.02	Joback Method
dvisc	0.0000492	Pa×s	780.35	Joback Method
dvisc	0.0000361	Pa×s	847.69	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=C55334753&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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