Eicosanyl propionate

Inchi: InChI=1S/C23H46O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-23(24)
InchiKey: OPEHDFRKFVXKNP-UHFFFAOYSA-N
Formula: C23H46O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)CC
Mol. weight [g/mol]: 354.61

Physical Properties

Property code	Value	Unit	Source
gf	-91.14	kJ/mol	Joback Method
hf	-762.85	kJ/mol	Joback Method
hfus	58.11	kJ/mol	Joback Method
hvap	75.95	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	7.981		Crippen Method
mcvol	342.370	ml/mol	McGowan Method
pc	875.32	kPa	Joback Method
rinpol	2490.00		NIST Webbook
tb	801.93	K	Joback Method
tc	982.34	K	Joback Method
tf	421.13	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.53	J/mol×K	801.93	Joback Method
cpg	1188.50	J/mol×K	952.27	Joback Method
cpg	1171.55	J/mol×K	922.21	Joback Method
cpg	1153.61	J/mol×K	892.14	Joback Method
cpg	1134.65	J/mol×K	862.07	Joback Method
cpg	1114.64	J/mol×K	832.00	Joback Method
cpg	1204.49	J/mol×K	982.34	Joback Method
dvisc	0.0000483	Pa×s	801.93	Joback Method
dvisc	0.0000655	Pa×s	738.46	Joback Method

dvisc	0.0000941	Pa×s	675.00	Joback Method
dvisc	0.0001457	Pa×s	611.53	Joback Method
dvisc	0.0002498	Pa×s	548.06	Joback Method
dvisc	0.0004928	Pa×s	484.60	Joback Method
dvisc	0.0011936	Pa×s	421.13	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=R543018&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