Eicosyl butyrate

Inchi: InChI=1S/C24H48O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23-26-24(25
InchiKey: KXZTZTCVTSKMMY-UHFFFAOYSA-N
Formula: C24H48O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)CCC
Mol. weight [g/mol]: 368.64

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	2579.00		NIST Webbook
rinpol	2574.00		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/mol×K	824.81	Joback Method
cpg	1178.47	J/mol×K	855.64	Joback Method
cpg	1198.97	J/mol×K	886.48	Joback Method
cpg	1218.34	J/mol×K	917.31	Joback Method
cpg	1236.63	J/mol×K	948.14	Joback Method
cpg	1253.86	J/mol×K	978.97	Joback Method
cpg	1270.08	J/mol×K	1009.81	Joback Method
dvisc	0.0010603	Pa×s	432.40	Joback Method

dvisc	0.0004342	Pa×s	497.80	Joback Method
dvisc	0.0002188	Pa×s	563.20	Joback Method
dvisc	0.0001271	Pa×s	628.61	Joback Method
dvisc	0.0000818	Pa×s	694.01	Joback Method
dvisc	0.0000568	Pa×s	759.41	Joback Method
dvisc	0.0000418	Pa×s	824.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R399272&Units=SI
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

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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