2-Monolinolenin

Other names: 2-Monolinolenin
Inchi: InChI=1S/C21H36O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21(24)25-19-20(23)18
InchiKey: GGJRAQULURVTAJ-PDBXOOCHSA-N
Formula: C21H36O4
SMILES: CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)OCC(O)CO
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
hfus	58.19	kJ/mol	Joback Method
hvap	143.24	kJ/mol	Cheméo Relay (1.0)
logp	4.472		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
rinpol	2161.00		NIST Webbook
rinpol	2161.00		NIST Webbook
tb	654.10	K	Cheméo Relay (1.0)
tc	856.60	K	Cheméo Relay (1.0)
tf	300.86	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.76	J/mol×K	952.57	Joback Method
cpg	1124.75	J/mol×K	1170.58	Joback Method
cpg	1111.13	J/mol×K	1134.24	Joback Method
cpg	1097.09	J/mol×K	1097.91	Joback Method
cpg	1082.53	J/mol×K	1061.57	Joback Method
cpg	1067.35	J/mol×K	1025.24	Joback Method
cpg	1051.46	J/mol×K	988.90	Joback Method
dvisc	0.0000053	Pa×s	721.28	Joback Method
dvisc	0.0000007	Pa×s	952.57	Joback Method
dvisc	0.0000012	Pa×s	875.47	Joback Method
dvisc	0.0000023	Pa×s	798.38	Joback Method
dvisc	0.0002781	Pa×s	489.99	Joback Method

dvisc	0.0000144	Pa×s	644.18	Joback Method
dvisc	0.0000517	Pa×s	567.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55268581&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point