3-(Icosyloxy)propane-1,2-diol

Inchi: InChI=1S/C23H48O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-26-22-23(25
InchiKey: IKSHIHFYUOTYKW-UHFFFAOYSA-N
Formula: C23H48O3
SMILES: CCCCCCCCCCCCCCCCCCCCCOCC(O)CO
Mol. weight [g/mol]: 372.63
CAS: 10431-04-6

Physical Properties

Property code	Value	Unit	Source
gf	-238.30	kJ/mol	Joback Method
hf	-960.01	kJ/mol	Joback Method
hfus	61.17	kJ/mol	Joback Method
hvap	102.17	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.398		Crippen Method
mcvol	352.540	ml/mol	McGowan Method
pc	946.16	kPa	Joback Method
rinpol	2817.90		NIST Webbook
rinpol	2817.90		NIST Webbook
tb	931.98	K	Joback Method
tc	1158.13	K	Joback Method
tf	477.84	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1224.61	J/mol×K	931.98	Joback Method
cpg	1246.09	J/mol×K	969.67	Joback Method
cpg	1266.10	J/mol×K	1007.36	Joback Method
cpg	1284.70	J/mol×K	1045.06	Joback Method
cpg	1301.96	J/mol×K	1082.75	Joback Method
cpg	1317.97	J/mol×K	1120.44	Joback Method
cpg	1332.78	J/mol×K	1158.13	Joback Method

dvisc	0.0004186	Pa×s	477.84	Joback Method
dvisc	0.0000736	Pa×s	553.53	Joback Method
dvisc	0.0000197	Pa×s	629.22	Joback Method
dvisc	0.0000070	Pa×s	704.91	Joback Method
dvisc	0.0000030	Pa×s	780.60	Joback Method
dvisc	0.0000015	Pa×s	856.29	Joback Method
dvisc	0.0000009	Pa×s	931.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10431046&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