

Span 60

Inchi: InChI=1S/C24H46O6/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22(27)29-19-21(26)24-23-20-18-22
InchiKey: HVUMOYIDDBPOLL-UHFFFAOYSA-N
Formula: C24H46O6
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCC(O)C1OCC(O)C1O
Mol. weight [g/mol]: 430.63
CAS: 1338-41-6

Physical Properties

Property code	Value	Unit	Source
hf	-1349.68	kJ/mol	Cheméo Relay (1.0)
hfus	75.08	kJ/mol	Joback Method
hvap	166.61	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.51		Cheméo Relay (1.0)
logp	4.273		Crippen Method
mcvol	369.080	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
tb	710.08	K	Cheméo Relay (1.0)
tc	925.68	K	Cheméo Relay (1.0)
tf	329.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-1.06130e+01
Coeff. B	2.41262e+00
Coeff. C	-1.28430e-03
Coeff. D	2.20600e-07
Coeff. E	0.00000e+00
Basis	predicted

Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	$Y = \exp(A + B/T + C \cdot \ln(T) + D \cdot T^E)$
Y unit	Pa·s
Coeff. A	-2.31868e+01
Coeff. B	7.79898e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	329.15
Temperature range (K), max.	1003.60

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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