

Etoglucid

Inchi:	InChI=1S/C12H22O6/c1(13-3-5-15-7-11-9-17-11)2-14-4-6-16-8-12-10-18-12/h11-12H,1-
InchiKey:	UMILHIMHKXVDGH-UHFFFAOYSA-N
Formula:	C12H22O6
SMILES:	C(COCCOCC1CO1)OCCOCC1CO1
Mol. weight [g/mol]:	262.30
CAS:	1954-28-5

Physical Properties

Property code	Value	Unit	Source
hf	-887.57	kJ/mol	Cheméo Relay (1.0)
hfus	43.82	kJ/mol	Joback Method
hvap	90.85	kJ/mol	Cheméo Relay (1.0)
ie	9.58	eV	Cheméo Relay (1.0)
logp	-0.150		Crippen Method
mcvol	193.440	ml/mol	McGowan Method
tb	606.92	K	Cheméo Relay (1.0)
tf	260.15	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	2.81380e+01
Coeff. B	1.18680e+00
Coeff. C	-5.97600e-04
Coeff. D	9.36000e-08
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	-9.76850e+00
Coeff. B	1.35078e+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 T_f to $0.7 \cdot T_c$.
Temperature range (K), min.	260.15
Temperature range (K), max.	568.84

Sources

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):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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