3-Hexyne-2,5-diol

Other names: Hexyne-3-diol-2,5
3-Hexyn-2,5-diol
hex-3-yne-2,5-diol
Inchi: InChI=1S/C6H10O2/c1-5(7)3-4-6(2)8/h5-8H,1-2H3
InchiKey: KDOWHHULNTXTNS-UHFFFAOYSA-N
Formula: C6H10O2
SMILES: CC(O)C#CC(C)O
Mol. weight [g/mol]: 114.14
CAS: 3031-66-1

Physical Properties

Property code	Value	Unit	Source
gf	-76.08	kJ/mol	Joback Method
hf	-209.89	kJ/mol	Joback Method
hfus	15.55	kJ/mol	Joback Method
hvap	63.68	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	-0.249		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	4862.97	kPa	Joback Method
rinpol	161.40		NIST Webbook
rinpol	161.40		NIST Webbook
tb	529.16	K	Joback Method
tc	710.97	K	Joback Method
tf	355.12	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.64	J/mol×K	529.16	Joback Method
cpg	227.30	J/mol×K	559.46	Joback Method
cpg	234.63	J/mol×K	589.76	Joback Method
cpg	241.64	J/mol×K	620.06	Joback Method

cpg	248.34	J/mol×K	650.36	Joback Method
cpg	254.74	J/mol×K	680.66	Joback Method
cpg	260.84	J/mol×K	710.97	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.20	K	2.00	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3031661&Units=SI

Legend

cpg: Ideal gas heat capacity
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume