3,5-Dimethyl-4-heptanol

Inchi: InChI=1S/C9H20O/c1-5-7(3)9(10)8(4)6-2/h7-10H,5-6H2,1-4H3
InchiKey: ZKXITRNXHWEQJU-UHFFFAOYSA-N
Formula: C9H20O
SMILES: CCC(C)C(O)C(C)CC
Mol. weight [g/mol]: 144.26
CAS: 19549-79-2

Physical Properties

Property code	Value	Unit	Source
af	0.5829		Cheméo Relay (1.0)
gf	-119.24	kJ/mol	Joback Method
hf	-401.57	kJ/mol	Cheméo Relay (1.0)
hfus	12.58	kJ/mol	Joback Method
hvap	61.13	kJ/mol	Cheméo Relay (1.0)
ie	9.39	eV	Cheméo Relay (1.0)
log10ws	-2.17		Cheméo Relay (1.0)
logp	2.440		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
tb	448.61	K	Cheméo Relay (1.0)
tc	635.08	K	Cheméo Relay (1.0)
tf	231.75	K	Cheméo Relay (1.0)
vc	0.509	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.97	J/mol×K	496.18	Joback Method
cpg	348.32	J/mol×K	524.25	Joback Method
cpg	361.14	J/mol×K	552.32	Joback Method
cpg	373.44	J/mol×K	580.39	Joback Method
cpg	385.22	J/mol×K	608.46	Joback Method
cpg	396.50	J/mol×K	636.53	Joback Method
cpg	407.30	J/mol×K	664.60	Joback Method

dvisc	0.5757064	Pa×s	207.01	Joback Method
dvisc	0.0376026	Pa×s	255.20	Joback Method
dvisc	0.0058439	Pa×s	303.40	Joback Method
dvisc	0.0015130	Pa×s	351.59	Joback Method
dvisc	0.0005426	Pa×s	399.79	Joback Method
dvisc	0.0002426	Pa×s	447.98	Joback Method
dvisc	0.0001269	Pa×s	496.18	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73855e+01
Coeff. B	-4.89083e+03
Coeff. C	-6.90720e+01
Temperature range (K), min.	355.12
Temperature range (K), max.	474.14

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):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19549792&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume