4-Heptanol, 2,4,6-trimethyl-

Other names: 2,4,6-Trimethyl-4-heptanol
Inchi: InChI=1S/C10H22O/c1-8(2)6-10(5,11)7-9(3)4/h8-9,11H,6-7H2,1-5H3
InchiKey: QSVYJSJPLCSACO-UHFFFAOYSA-N
Formula: C10H22O
SMILES: CC(C)CC(C)(O)CC(C)C
Mol. weight [g/mol]: 158.28
CAS: 60836-07-9

Physical Properties

Property code	Value	Unit	Source
gf	-105.54	kJ/mol	Joback Method
hf	-421.27	kJ/mol	Joback Method
hfus	11.28	kJ/mol	Joback Method
hvap	52.46	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.830		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
tb	516.27	K	Joback Method
tc	689.38	K	Joback Method
tf	235.70	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.00	J/mol×K	516.27	Joback Method
cpg	398.75	J/mol×K	545.12	Joback Method
cpg	412.80	J/mol×K	573.97	Joback Method
cpg	426.18	J/mol×K	602.82	Joback Method
cpg	438.91	J/mol×K	631.67	Joback Method
cpg	451.03	J/mol×K	660.53	Joback Method
cpg	462.55	J/mol×K	689.38	Joback Method
dvisc	0.2106679	Pa×s	235.70	Joback Method

dvisc	0.0209261	Pa×s	282.46	Joback Method
dvisc	0.0040057	Pa×s	329.22	Joback Method
dvisc	0.0011568	Pa×s	375.99	Joback Method
dvisc	0.0004397	Pa×s	422.75	Joback Method
dvisc	0.0002027	Pa×s	469.51	Joback Method
dvisc	0.0001075	Pa×s	516.27	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	454.20	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64121e+01
Coeff. B	-4.57030e+03
Coeff. C	-6.76820e+01
Temperature range (K), min.	351.12
Temperature range (K), max.	479.40

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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=C60836079&Units=SI

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume