3,4-dimethyloctane, threo

Inchi: InChI=1S/C10H22/c1-5-7-8-10(4)9(3)6-2/h9-10H,5-8H2,1-4H3/t9-,10-/m1/s1
InchiKey: QQCWGAMGBCGAQJ-NXEZZACHSA-N
Formula: C10H22
SMILES: CCCCC(C)C(C)CC
Mol. weight [g/mol]: 142.28

Physical Properties

Property code	Value	Unit	Source
gf	28.44	kJ/mol	Joback Method
hf	-260.29	kJ/mol	Joback Method
hfus	14.61	kJ/mol	Joback Method
hvap	37.08	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.859		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	936.30		NIST Webbook
rinpol	936.30		NIST Webbook
rinpol	954.00		NIST Webbook
tb	427.32	K	Joback Method
tc	596.92	K	Joback Method
tf	172.46	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.26	J/mol×K	427.32	Joback Method
cpg	331.18	J/mol×K	455.59	Joback Method
cpg	346.50	J/mol×K	483.85	Joback Method
cpg	361.21	J/mol×K	512.12	Joback Method
cpg	375.35	J/mol×K	540.39	Joback Method
cpg	388.93	J/mol×K	568.65	Joback Method
cpg	401.95	J/mol×K	596.92	Joback Method

dvisc	0.0214146	Pa×s	172.46	Joback Method
dvisc	0.0046771	Pa×s	214.94	Joback Method
dvisc	0.0016877	Pa×s	257.41	Joback Method
dvisc	0.0008129	Pa×s	299.89	Joback Method
dvisc	0.0004693	Pa×s	342.37	Joback Method
dvisc	0.0003059	Pa×s	384.84	Joback Method
dvisc	0.0002171	Pa×s	427.32	Joback Method

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=R293411&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume