

3,5-dimethyloctane, threo

Inchi:	InChI=1S/C10H22/c1-5-7-10(4)8-9(3)6-2/h9-10H,5-8H2,1-4H3/t9-,10-/m1/s1
InchiKey:	VRHRGVJOUHJULC-NXEZZACHSA-N
Formula:	C10H22
SMILES:	CCCC(C)CC(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	922.00		NIST Webbook
rinpol	922.00		NIST Webbook
tb	427.32	K	Joback Method
tc	596.92	K	Joback Method
tf	172.46	K	Joback Method
vc	0.584	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.26	J/mol×K	427.32	Joback Method
cpg	388.93	J/mol×K	568.65	Joback Method
cpg	375.35	J/mol×K	540.39	Joback Method
cpg	361.21	J/mol×K	512.12	Joback Method
cpg	346.50	J/mol×K	483.85	Joback Method
cpg	331.18	J/mol×K	455.59	Joback Method
cpg	401.95	J/mol×K	596.92	Joback Method
dvisc	0.0002171	Paxs	427.32	Joback Method

dvisc	0.0003059	Paxs	384.84	Joback Method
dvisc	0.0004693	Paxs	342.37	Joback Method
dvisc	0.0008129	Paxs	299.89	Joback Method
dvisc	0.0016877	Paxs	257.41	Joback Method
dvisc	0.0046771	Paxs	214.94	Joback Method
dvisc	0.0214146	Paxs	172.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R293451&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

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