Heptane, 2,3,4-trimethyl-, erythro

Inchi: InChI=1S/C10H22/c1-6-7-9(4)10(5)8(2)3/h8-10H,6-7H2,1-5H3/t9-,10+/m0/s1
InchiKey: UVVYAKOLFKEZEE-VHSXEESVSA-N
Formula: C10H22
SMILES: CCCC(C)C(C)C(C)C
Mol. weight [g/mol]: 142.28

Physical Properties

Property code	Value	Unit	Source
gf	26.00	kJ/mol	Joback Method
hf	-265.57	kJ/mol	Joback Method
hfus	11.09	kJ/mol	Joback Method
hvap	36.69	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	3.715		Crippen Method
mcvol	151.760	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	933.70		NIST Webbook
rinpol	933.70		NIST Webbook
tb	426.88	K	Joback Method
tc	600.24	K	Joback Method
tf	157.46	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.23	J/mol×K	426.88	Joback Method
cpg	331.59	J/mol×K	455.77	Joback Method
cpg	347.31	J/mol×K	484.67	Joback Method
cpg	362.39	J/mol×K	513.56	Joback Method
cpg	376.87	J/mol×K	542.45	Joback Method
cpg	390.75	J/mol×K	571.35	Joback Method
cpg	404.05	J/mol×K	600.24	Joback Method
dvisc	0.0495825	Pa×s	157.46	Joback Method

dvisc	0.0072381	Pa×s	202.36	Joback Method
dvisc	0.0021254	Pa×s	247.27	Joback Method
dvisc	0.0009096	Pa×s	292.17	Joback Method
dvisc	0.0004880	Pa×s	337.07	Joback Method
dvisc	0.0003031	Pa×s	381.98	Joback Method
dvisc	0.0002081	Pa×s	426.88	Joback Method

Sources

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=R294805&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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