3,4,7-Trimethylnonane, d

Inchi: InChI=1S/C12H26/c1-6-10(3)8-9-12(5)11(4)7-2/h10-12H,6-9H2,1-5H3
InchiKey: HQIBDLHPQGDJEW-UHFFFAOYSA-N
Formula: C12H26
SMILES: CCC(C)CCC(C)C(C)CC
Mol. weight [g/mol]: 170.33

Physical Properties

Property code	Value	Unit	Source
gf	42.84	kJ/mol	Joback Method
hf	-306.85	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	41.14	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	4.495		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	1116.60		NIST Webbook
tb	472.64	K	Joback Method
tc	643.64	K	Joback Method
tf	180.00	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.03	J/mol×K	472.64	Joback Method
cpg	490.12	J/mol×K	615.14	Joback Method
cpg	474.87	J/mol×K	586.64	Joback Method
cpg	458.95	J/mol×K	558.14	Joback Method
cpg	442.35	J/mol×K	529.64	Joback Method
cpg	425.05	J/mol×K	501.14	Joback Method
cpg	504.72	J/mol×K	643.64	Joback Method
dvisc	0.0001829	Pa×s	472.64	Joback Method
dvisc	0.0002670	Pa×s	423.87	Joback Method

dvisc	0.0004300	Pa×s	375.09	Joback Method
dvisc	0.0007987	Pa×s	326.32	Joback Method
dvisc	0.0018440	Pa×s	277.55	Joback Method
dvisc	0.0060831	Pa×s	228.77	Joback Method
dvisc	0.0383167	Pa×s	180.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R173347&Units=SI
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

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