4,5-dimethyl-2,3-diethylheptane

Inchi: InChI=1S/C13H28/c1-7-10(4)12(6)13(9-3)11(5)8-2/h10-13H,7-9H2,1-6H3
InchiKey: HZHQAPYQJPNACQ-UHFFFAOYSA-N
Formula: C13H28
SMILES: CCC(C)C(C)C(CC)C(C)CC
Mol. weight [g/mol]: 184.36

Physical Properties

Property code	Value	Unit	Source
gf	48.82	kJ/mol	Joback Method
hf	-332.77	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	42.98	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.741		Crippen Method
mcvol	194.030	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	936.00		NIST Webbook
rinpol	936.00		NIST Webbook
tb	495.08	K	Joback Method
tc	668.26	K	Joback Method
tf	176.27	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.92	J/mol×K	495.08	Joback Method
cpg	475.07	J/mol×K	523.94	Joback Method
cpg	493.42	J/mol×K	552.81	Joback Method
cpg	511.01	J/mol×K	581.67	Joback Method
cpg	527.85	J/mol×K	610.53	Joback Method
cpg	543.96	J/mol×K	639.40	Joback Method
cpg	559.36	J/mol×K	668.26	Joback Method
dvisc	0.0754463	Pa×s	176.27	Joback Method

dvisc	0.0082339	Pa×s	229.41	Joback Method
dvisc	0.0020674	Pa×s	282.54	Joback Method
dvisc	0.0008040	Pa×s	335.67	Joback Method
dvisc	0.0004047	Pa×s	388.81	Joback Method
dvisc	0.0002403	Pa×s	441.94	Joback Method
dvisc	0.0001596	Pa×s	495.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R306062&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