3-methyl, 3,5-diethyl, heptane

Inchi: InChI=1S/C12H26/c1-6-11(7-2)10-12(5,8-3)9-4/h11H,6-10H2,1-5H3
InchiKey: RGRSPNWZJFXFAN-UHFFFAOYSA-N
Formula: C12H26
SMILES: CCC(CC)CC(C)(CC)CC
Mol. weight [g/mol]: 170.33

Physical Properties

Property code	Value	Unit	Source
gf	50.56	kJ/mol	Joback Method
hf	-305.04	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	40.62	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.639		Crippen Method
mcvol	179.940	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	1112.40		NIST Webbook
rinpol	1112.40		NIST Webbook
tb	470.29	K	Joback Method
tc	644.11	K	Joback Method
tf	212.42	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.02	J/mol×K	470.29	Joback Method
cpg	427.54	J/mol×K	499.26	Joback Method
cpg	445.22	J/mol×K	528.23	Joback Method
cpg	462.09	J/mol×K	557.20	Joback Method
cpg	478.18	J/mol×K	586.17	Joback Method
cpg	493.52	J/mol×K	615.14	Joback Method
cpg	508.14	J/mol×K	644.11	Joback Method
dvisc	0.0170934	Pa×s	212.42	Joback Method

dvisc	0.0043803	Pa×s	255.40	Joback Method
dvisc	0.0016616	Pa×s	298.38	Joback Method
dvisc	0.0008046	Pa×s	341.36	Joback Method
dvisc	0.0004582	Pa×s	384.33	Joback Method
dvisc	0.0002922	Pa×s	427.31	Joback Method
dvisc	0.0002023	Pa×s	470.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R173387&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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