

3,7,11-trimethyl-6-(3-methylpentyl)tridecane

Inchi: InChI=1S/C22H46/c1-8-18(4)12-11-13-21(7)22(16-14-19(5)9-2)17-15-20(6)10-3/h18-22H
InchiKey: AWXYDFNLHZBEOR-UHFFFAOYSA-N
Formula: C22H46
SMILES: CCC(C)CCCC(C)C(CCC(C)CC)CCC(C)CC
Mol. weight [g/mol]: 310.60

Physical Properties

Property code	Value	Unit	Source
gf	122.16	kJ/mol	Joback Method
hf	-523.81	kJ/mol	Joback Method
hfus	35.12	kJ/mol	Joback Method
hvap	62.63	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	8.108		Crippen Method
mcvol	320.840	ml/mol	McGowan Method
pc	923.86	kPa	Joback Method
rinpol	1901.00		NIST Webbook
tb	700.56	K	Joback Method
tc	871.25	K	Joback Method
tf	262.70	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.84	J/mol×K	700.56	Joback Method
cpg	986.71	J/mol×K	729.01	Joback Method
cpg	1008.54	J/mol×K	757.46	Joback Method
cpg	1029.35	J/mol×K	785.91	Joback Method
cpg	1049.19	J/mol×K	814.36	Joback Method
cpg	1068.08	J/mol×K	842.80	Joback Method
cpg	1086.07	J/mol×K	871.25	Joback Method
dvisc	0.0231814	Pa×s	262.70	Joback Method
dvisc	0.0027611	Pa×s	335.68	Joback Method

dvisc	0.0007032	Pa×s	408.65	Joback Method
dvisc	0.0002710	Pa×s	481.63	Joback Method
dvisc	0.0001343	Pa×s	554.61	Joback Method
dvisc	0.0000783	Pa×s	627.58	Joback Method
dvisc	0.0000511	Pa×s	700.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R261964&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

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