

2,6,10-trimethyl-7-(3-methylpentyl)dodecane

Inchi:	InChI=1S/C21H44/c1-8-18(5)13-15-21(16-14-19(6)9-2)20(7)12-10-11-17(3)4/h17-21H,8-
InchiKey:	XKRXQMYLJXTKHC-UHFFFAOYSA-N
Formula:	C21H44
SMILES:	CCC(C)CCC(CCC(C)CC)C(C)CCCC(C)C
Mol. weight [g/mol]:	296.57

Physical Properties

Property code	Value	Unit	Source
gf	113.74	kJ/mol	Joback Method
hf	-503.17	kJ/mol	Joback Method
hfus	32.53	kJ/mol	Joback Method
hvap	60.40	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	7.718		Crippen Method
mcvol	306.750	ml/mol	McGowan Method
pc	980.23	kPa	Joback Method
rinpol	1801.00		NIST Webbook
tb	677.68	K	Joback Method
tc	847.67	K	Joback Method
tf	251.43	K	Joback Method
vc	1.181	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.47	J/molxK	677.68	Joback Method
cpg	1005.61	J/molxK	819.34	Joback Method
cpg	986.89	J/molxK	791.01	Joback Method
cpg	967.25	J/molxK	762.68	Joback Method
cpg	946.65	J/molxK	734.34	Joback Method
cpg	925.07	J/molxK	706.01	Joback Method
cpg	1023.44	J/molxK	847.67	Joback Method
dvisc	0.0000587	Paxs	677.68	Joback Method
dvisc	0.0000900	Paxs	606.64	Joback Method

dvisc	0.0001547	Paxs	535.60	Joback Method
dvisc	0.0003138	Paxs	464.56	Joback Method
dvisc	0.0008215	Paxs	393.51	Joback Method
dvisc	0.0032873	Paxs	322.47	Joback Method
dvisc	0.0287988	Paxs	251.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R261944&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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