Cyclohexane, 1-(3,7-dimethylnonyl)-2,2,6-trimethyl, # 2

Inchi: InChI=1S/C21H42/c1-7-10-17(2)11-8-12-18(3)14-15-20-19(4)13-9-16-21(20,5)6/h17-20H

InchiKey: DAMPNNUACKJWFF-UHFFFAOYSA-N

Formula: C21H42

SMILES: CCCC(C)CCCC(C)CCC1C(C)CCCC1(C)C

Mol. weight [g/mol]: 294.56

Physical Properties

Property code	Value	Unit	Source
gf	124.60	kJ/mol	Joback Method
hf	-458.45	kJ/mol	Joback Method
hfus	30.78	kJ/mol	Joback Method
hvap	60.22	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	7.472		Crippen Method
mcvol	295.890	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
rinpol	1841.00		NIST Webbook
rinpol	1841.00		NIST Webbook
tb	689.45	K	Joback Method
tc	876.65	K	Joback Method
tf	319.23	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.36	J/mol×K	689.45	Joback Method
cpg	923.50	J/mol×K	720.65	Joback Method
cpg	947.52	J/mol×K	751.85	Joback Method
cpg	970.52	J/mol×K	783.05	Joback Method
cpg	992.59	J/mol×K	814.25	Joback Method
cpg	1013.81	J/mol×K	845.45	Joback Method
cpg	1034.28	J/mol×K	876.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R553703&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
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