3,7,11,15-Tetramethyl-2-hexadecen-1-al

Inchi: InChI=1S/C20H38O/c1-17(2)9-6-10-18(3)11-7-12-19(4)13-8-14-20(5)15-16-21/h15-19H,6

InchiKey: RAFZYSUICBQABU-HMMYKYKNSA-N

Formula: C20H38O

SMILES: CC(=CC=O)CCCC(C)CCCC(C)CCCC(C)C

Mol. weight [g/mol]: 294.52

Physical Properties

Property code	Value	Unit	Source
gf	82.35	kJ/mol	Joback Method
hf	-450.12	kJ/mol	Joback Method
hfus	38.17	kJ/mol	Joback Method
hvap	65.71	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	6.571		Crippen Method
mcvol	289.930	ml/mol	McGowan Method
pc	1123.81	kPa	Joback Method
rinpol	2189.00		NIST Webbook
tb	708.38	K	Joback Method
tc	885.64	K	Joback Method
tf	293.12	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.75	J/mol×K	708.38	Joback Method
cpg	872.72	J/mol×K	737.92	Joback Method
cpg	891.73	J/mol×K	767.47	Joback Method
cpg	909.82	J/mol×K	797.01	Joback Method
cpg	927.04	J/mol×K	826.55	Joback Method
cpg	943.42	J/mol×K	856.09	Joback Method
cpg	959.01	J/mol×K	885.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R528400&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
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