6-Methyl-4,6-bis(4-methylpent-3-en-1-yl)cyclohexa

Inchi: InChI=1S/C20H30O/c1-16(2)8-6-10-18-11-12-19(15-21)20(5,14-18)13-7-9-17(3)4/h8-9,1
InchiKey: FENFKJSEQOAPKE-UHFFFAOYSA-N
Formula: C20H30O
SMILES: CC(C)=CCCC1=CC=C(C=O)C(C)(CCC=C(C)C)C1
Mol. weight [g/mol]: 286.45
CAS: 61447-89-0

Physical Properties

Property code	Value	Unit	Source
gf	220.96	kJ/mol	Joback Method
hf	-164.67	kJ/mol	Joback Method
hfus	34.83	kJ/mol	Joback Method
hvap	68.10	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.941		Crippen Method
mcvol	266.170	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2113.40		NIST Webbook
tb	741.81	K	Joback Method
tc	950.22	K	Joback Method
tf	376.92	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.78	J/mol×K	741.81	Joback Method
cpg	789.38	J/mol×K	776.55	Joback Method
cpg	808.23	J/mol×K	811.28	Joback Method
cpg	826.47	J/mol×K	846.02	Joback Method
cpg	844.27	J/mol×K	880.75	Joback Method
cpg	861.75	J/mol×K	915.49	Joback Method
cpg	879.09	J/mol×K	950.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61447890&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