(E)-1-(6,10-Dimethylundec-5-en-2-yl)-4-methylben

Inchi: InChI=1S/C20H32/c1-16(2)8-6-9-17(3)10-7-11-19(5)20-14-12-18(4)13-15-20/h10,12-16,1
InchiKey: NUBCIXDDSVLPIU-LICLKQGHSA-N
Formula: C20H32
SMILES: CC(=CCCC(C)c1ccc(C)cc1)CCCC(C)C
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
gf	287.09	kJ/mol	Joback Method
hf	-134.20	kJ/mol	Joback Method
hfus	33.05	kJ/mol	Joback Method
hvap	62.31	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.651		Crippen Method
mcvol	264.600	ml/mol	McGowan Method
pc	1323.28	kPa	Joback Method
rinpol	1910.00		NIST Webbook
rinpol	1991.80		NIST Webbook
rinpol	1910.00		NIST Webbook
ripol	2267.00		NIST Webbook
tb	691.82	K	Joback Method
tc	890.00	K	Joback Method
tf	305.06	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.00	J/mol×K	691.82	Joback Method
cpg	766.62	J/mol×K	724.85	Joback Method
cpg	786.10	J/mol×K	757.88	Joback Method
cpg	804.50	J/mol×K	790.91	Joback Method
cpg	821.88	J/mol×K	823.94	Joback Method
cpg	838.31	J/mol×K	856.97	Joback Method

cpg	853.83	J/mol×K	890.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume