(4aS,4bS,10aS)-1,1,4a-Trimethyl-7-(propan-2-ylide

Inchi: InChI=1S/C20H32/c1-14(2)15-7-9-17-16(13-15)8-10-18-19(3,4)11-6-12-20(17,18)5/h13,1
InchiKey: MRRHSEMHYVQUFK-GGPKGHCWSA-N
Formula: C20H32
SMILES: CC(C)=C1C=C2CCC3C(C)(C)CCCC3(C)C2CC1
Mol. weight [g/mol]: 272.47
CAS: 57119-12-7

Physical Properties

Property code	Value	Unit	Source
gf	277.82	kJ/mol	Joback Method
hf	-145.84	kJ/mol	Joback Method
hfus	19.78	kJ/mol	Joback Method
hvap	59.92	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.286		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2170.90		NIST Webbook
rinpol	2170.90		NIST Webbook
tb	705.04	K	Joback Method
tc	941.51	K	Joback Method
tf	404.62	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.59	J/mol×K	705.04	Joback Method
cpg	792.65	J/mol×K	744.45	Joback Method
cpg	817.69	J/mol×K	783.86	Joback Method
cpg	842.05	J/mol×K	823.27	Joback Method
cpg	866.08	J/mol×K	862.68	Joback Method
cpg	890.10	J/mol×K	902.10	Joback Method
cpg	914.46	J/mol×K	941.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57119127&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