(4aS,4bS,10aS)-7-Isopropyl-1,1,4a-trimethyl-1,2,3,

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/h7,13
InchiKey: ASPVQUYRFYUDSC-GGPKGHCWSA-N
Formula: C20H32
SMILES: CC(C)C1=CCC2C(=C1)CCC1C(C)(C)CCCC21C
Mol. weight [g/mol]: 272.47
CAS: 122712-77-0

Physical Properties

Property code	Value	Unit	Source
gf	258.80	kJ/mol	Joback Method
hf	-171.05	kJ/mol	Joback Method
hfus	18.08	kJ/mol	Joback Method
hvap	59.62	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	6.142		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
rinpol	2039.80		NIST Webbook
rinpol	2039.80		NIST Webbook
tb	702.22	K	Joback Method
tc	935.86	K	Joback Method
tf	406.50	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.28	J/mol×K	702.22	Joback Method
cpg	792.08	J/mol×K	741.16	Joback Method
cpg	816.84	J/mol×K	780.10	Joback Method
cpg	840.88	J/mol×K	819.04	Joback Method
cpg	864.52	J/mol×K	857.98	Joback Method
cpg	888.08	J/mol×K	896.92	Joback Method
cpg	911.87	J/mol×K	935.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122712770&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