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

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: KEQXEEMBFONZBL-QUCCMNQESA-N
Formula: C20H32
SMILES: CC(C)C1=CC2=C(CC1)C1(C)CCCC(C)(C)C1CC2
Mol. weight [g/mol]: 272.47
CAS: 41577-36-0

Physical Properties

Property code	Value	Unit	Source
gf	256.88	kJ/mol	Joback Method
hf	-162.18	kJ/mol	Joback Method
hfus	16.62	kJ/mol	Joback Method
hvap	60.59	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.286		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	2035.60		NIST Webbook
rinpol	2035.60		NIST Webbook
ripol	2489.00		NIST Webbook
ripol	2489.00		NIST Webbook
ripol	2489.00		NIST Webbook
tb	711.87	K	Joback Method
tc	946.21	K	Joback Method
tf	423.26	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.74	J/mol×K	711.87	Joback Method
cpg	789.91	J/mol×K	750.93	Joback Method
cpg	814.18	J/mol×K	789.98	Joback Method
cpg	837.86	J/mol×K	829.04	Joback Method

cpg	861.28	J/mol×K	868.09	Joback Method
cpg	884.76	J/mol×K	907.15	Joback Method
cpg	908.63	J/mol×K	946.21	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=C41577360&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

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