

Sandaracopimarinal

Inchi: InChI=1S/C20H30O/c1-5-18(2)12-9-16-15(13-18)7-8-17-19(3,14-21)10-6-11-20(16,17)4/
InchiKey: JKBKXKTXDKYEOR-WKXIVMOISA-N
Formula: C20H30O
SMILES: C=CC1(C)C=C2CCC3C(C)(C=O)CCCC3(C)C2CC1
Mol. weight [g/mol]: 286.45
CAS: 3855-14-9

Physical Properties

Property code	Value	Unit	Source
gf	216.03	kJ/mol	Joback Method
hf	-177.33	kJ/mol	Joback Method
hfus	16.55	kJ/mol	Joback Method
hvap	63.65	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.321		Crippen Method
mcvol	253.050	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2213.60		NIST Webbook
rinpol	2185.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2185.00		NIST Webbook
rinpol	2213.60		NIST Webbook
rinpol	2185.00		NIST Webbook
rinpol	2161.00		NIST Webbook
rinpol	2185.00		NIST Webbook
ripol	2785.00		NIST Webbook
ripol	2787.00		NIST Webbook
ripol	2785.00		NIST Webbook
tb	739.43	K	Joback Method
tc	979.37	K	Joback Method
tf	468.12	K	Joback Method
vc	0.963	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.90	J/molxK	739.43	Joback Method
cpg	816.13	J/molxK	779.42	Joback Method
cpg	841.06	J/molxK	819.41	Joback Method
cpg	866.16	J/molxK	859.40	Joback Method
cpg	891.89	J/molxK	899.39	Joback Method
cpg	918.71	J/molxK	939.38	Joback Method
cpg	947.09	J/molxK	979.37	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=C3855149&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
ripol:	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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