

(S)-3-Methyl-5-((1R,4aR,8aR)-5,5,8a-trimethyl-2-methyl-2-oxobicyclo[2.2.1]heptan-2-ylidene)pentanoic acid

InChI:
acid

InChI=1S/C20H34O2/c1-14(13-18(21)22)7-9-16-15(2)8-10-17-19(3,4)11-6-12-20(16,17)5

InChIKey:

NALGVVPRJHXHNM-UHFFFAOYSA-N

Formula:

C20H34O2

SMILES:

C=C1CCC2C(C)(C)CCCC2(C)C1CCC(C)CC(=O)O

Mol. weight [g/mol]:

306.48

CAS:

20784-69-4

Physical Properties

Property code	Value	Unit	Source
gf	-50.88	kJ/mol	Joback Method
hf	-531.22	kJ/mol	Joback Method
hfus	25.98	kJ/mol	Joback Method
hvap	80.90	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.676		Crippen Method
mvol	274.080	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	2297.40		NIST Webbook
rinpol	2297.40		NIST Webbook
tb	823.47	K	Joback Method
tc	1030.30	K	Joback Method
tf	485.71	K	Joback Method
vc	1.034	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.64	J/molxK	823.47	Joback Method
cpg	932.42	J/molxK	857.94	Joback Method
cpg	953.98	J/molxK	892.41	Joback Method
cpg	975.52	J/molxK	926.89	Joback Method
cpg	997.23	J/molxK	961.36	Joback Method
cpg	1019.33	J/molxK	995.83	Joback Method
cpg	1042.00	J/molxK	1030.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20784694&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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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