(S)-Ethyl 3-methyl-5-((1S,4aS,8aS)-5,5,8a-trimethyl-2-methy

Inchi: InChI=1S/C22H38O2/c1-7-24-20(23)15-16(2)9-11-18-17(3)10-12-19-21(4,5)13-8-14-22(1

InchiKey: HFJMFXMSXZVNBZ-FUOQNJDISA-N

Formula: C22H38O2

SMILES: C=C1CCC2C(C)(C)CCCC2(C)C1CCC(C)CC(=O)OCC

Mol. weight [g/mol]: 334.54

CAS: 613673-55-5

Physical Properties

Property code	Value	Unit	Source
gf	-2.22	kJ/mol	Joback Method
hf	-552.49	kJ/mol	Joback Method
hfus	28.26	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	6.155		Crippen Method
mcvol	302.260	ml/mol	McGowan Method
pc	1211.51	kPa	Joback Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	799.47	K	Joback Method
tc	1009.15	K	Joback Method
tf	469.66	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.82	J/mol×K	799.47	Joback Method
cpg	1012.43	J/mol×K	834.42	Joback Method
cpg	1036.50	J/mol×K	869.36	Joback Method
cpg	1060.22	J/mol×K	904.31	Joback Method
cpg	1083.81	J/mol×K	939.26	Joback Method
cpg	1107.44	J/mol×K	974.20	Joback Method
cpg	1131.34	J/mol×K	1009.15	Joback Method

Sources

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=C613673555&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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