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

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: YYDZORCXDQFCAQ-FUOQNJDISA-N

Formula: C22H38O2

SMILES: CCOC(=O)CC(C)CCC1C(C)=CCC2C(C)(C)CCCC12C

Mol. weight [g/mol]: 334.54

CAS: 613673-52-2

Physical Properties

Property code	Value	Unit	Source
gf	-34.97	kJ/mol	Joback Method
hf	-590.42	kJ/mol	Joback Method
hfus	30.25	kJ/mol	Joback Method
hvap	71.88	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	6.155		Crippen Method
mcvol	302.260	ml/mol	McGowan Method
pc	1213.20	kPa	Joback Method
rinpol	2338.90		NIST Webbook
tb	804.45	K	Joback Method
tc	1015.04	K	Joback Method
tf	469.26	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.98	J/mol×K	804.45	Joback Method
cpg	1013.54	J/mol×K	839.55	Joback Method
cpg	1037.61	J/mol×K	874.65	Joback Method
cpg	1061.39	J/mol×K	909.74	Joback Method
cpg	1085.07	J/mol×K	944.84	Joback Method
cpg	1108.88	J/mol×K	979.94	Joback Method
cpg	1133.00	J/mol×K	1015.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C613673522&Units=SI

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