Pentanoic acid, 1,7,7-trimethylbicyclo[2.2.1]hept-2-yl ester, endo-

Other names: Bornyl ester of n-pentanoic acid
Valeric acid, 2-bornyl ester, endo-
Bornyl valerate
«alpha»-Terpinyl ester of n-pentanoic acid
Bornyl pentanoate
endo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl valerate

Inchi: InChI=1S/C15H26O2/c1-5-6-7-13(16)17-12-10-11-8-9-15(12,4)14(11,2)3/h11-12H,5-10H

InchiKey: ILUAVCBOWYHFAI-UHFFFAOYSA-N

Formula: C15H26O2

SMILES: CCCCC(=O)OC1CC2CCC1(C)C2(C)C

Mol. weight [g/mol]: 238.37

CAS: 7549-41-9

Physical Properties

Property code	Value	Unit	Source
gf	-75.50	kJ/mol	Joback Method
hf	-468.49	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	55.22	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.935		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
tb	627.78	K	Joback Method
tc	833.26	K	Joback Method
tf	402.65	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.16	J/mol×K	627.78	Joback Method
cpg	613.03	J/mol×K	662.03	Joback Method
cpg	631.96	J/mol×K	696.27	Joback Method

cpg	650.15	J/mol×K	730.52	Joback Method
cpg	667.80	J/mol×K	764.77	Joback Method
cpg	685.10	J/mol×K	799.01	Joback Method
cpg	702.24	J/mol×K	833.26	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=C7549419&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume