Butanoic acid, 3-methyl-, 1,7,7-trimethylbicyclo[2.2.1]hept-2-yl ester, exo-

Other names: Isobornyl 3-methylbutanoate
exo-bornyl isovalerate
Bornyl 2-methylbutyrate

Inchi: InChI=1S/C15H26O2/c1-10(2)8-13(16)17-12-9-11-6-7-15(12,5)14(11,3)4/h10-12H,6-9H2

InchiKey: MPYYVGIJHREDBO-UHFFFAOYSA-N

Formula: C15H26O2

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

Mol. weight [g/mol]: 238.37

CAS: 7779-73-9

Physical Properties

Property code	Value	Unit	Source
gf	-77.94	kJ/mol	Joback Method
hf	-473.77	kJ/mol	Joback Method
hfus	17.59	kJ/mol	Joback Method
hvap	54.83	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.790		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1494.00		NIST Webbook
rinpol	1525.40		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1520.00		NIST Webbook
rinpol	1525.40		NIST Webbook
rinpol	1494.00		NIST Webbook
ripol	1729.00		NIST Webbook
ripol	1729.00		NIST Webbook
ripol	1729.00		NIST Webbook
tb	627.34	K	Joback Method
tc	836.82	K	Joback Method
tf	387.65	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.55	J/mol×K	627.34	Joback Method
cpg	613.85	J/mol×K	662.25	Joback Method
cpg	633.16	J/mol×K	697.17	Joback Method
cpg	651.71	J/mol×K	732.08	Joback Method
cpg	669.68	J/mol×K	766.99	Joback Method
cpg	687.30	J/mol×K	801.90	Joback Method
cpg	704.76	J/mol×K	836.82	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=C7779739&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume