

Valeric acid, 2,2,4-trimethyl-3-oxo-, tert-butyl ester

Inchi:	InChI=1S/C12H22O3/c1-8(2)9(13)12(6,7)10(14)15-11(3,4)5/h8H,1-7H3
InchiKey:	FXJMOZRQCUAZPE-UHFFFAOYSA-N
Formula:	C12H22O3
SMILES:	CC(C)C(=O)C(C)(C)C(=O)OC(C)(C)C
Mol. weight [g/mol]:	214.30
CAS:	4447-75-0

Physical Properties

Property code	Value	Unit	Source
gf	-309.44	kJ/mol	Joback Method
hf	-671.17	kJ/mol	Joback Method
hfus	12.87	kJ/mol	Joback Method
hvap	55.23	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.579		Crippen Method
mcvol	188.950	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
tb	597.22	K	Joback Method
tc	797.80	K	Joback Method
tf	336.93	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.27	J/molxK	597.22	Joback Method
cpg	511.81	J/molxK	630.65	Joback Method
cpg	527.36	J/molxK	664.08	Joback Method
cpg	541.96	J/molxK	697.51	Joback Method
cpg	555.65	J/molxK	730.94	Joback Method
cpg	568.48	J/molxK	764.37	Joback Method
cpg	580.50	J/molxK	797.80	Joback Method
dvisc	0.0040306	Paxs	336.93	Joback Method
dvisc	0.0016864	Paxs	380.31	Joback Method

dvisc	0.0008434	Paxs	423.69	Joback Method
dvisc	0.0004797	Paxs	467.08	Joback Method
dvisc	0.0003003	Paxs	510.46	Joback Method
dvisc	0.0002023	Paxs	553.84	Joback Method
dvisc	0.0001444	Paxs	597.22	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4447750&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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