

n-Butyl tiglate

Other names:	2-Butenoic acid, 2-methyl-, butyl ester, (E)- Butyl tiglate Butyl «alpha»-methylcrotonate Tiglic acid n-butyl ester Butyl (E)-2-methylbut-2-enoate Butyl 2-methyl-2-butenate butyl 2-methylcrotonate
Inchi:	InChI=1S/C9H16O2/c1-4-6-7-11-9(10)8(3)5-2/h5H,4,6-7H2,1-3H3/b8-5+
InchiKey:	RBGFLIOXJWFKKX-VMPITWQZSA-N
Formula:	C9H16O2
SMILES:	CC=C(C)C(=O)OCCCC
Mol. weight [g/mol]:	156.22
CAS:	7785-66-2

Physical Properties

Property code	Value	Unit	Source
gf	-137.35	kJ/mol	Joback Method
hf	-366.46	kJ/mol	Joback Method
hfus	20.74	kJ/mol	Joback Method
hvap	44.82	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1136.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1419.00		NIST Webbook
tb	485.65	K	Joback Method
tc	670.48	K	Joback Method
tf	244.31	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.90	J/mol×K	485.65	Joback Method
cpg	319.01	J/mol×K	516.46	Joback Method
cpg	331.57	J/mol×K	547.26	Joback Method
cpg	343.57	J/mol×K	578.07	Joback Method
cpg	355.04	J/mol×K	608.87	Joback Method
cpg	365.99	J/mol×K	639.68	Joback Method
cpg	376.43	J/mol×K	670.48	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=C7785662&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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