

3-Tigloyloxynortropane

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C12H19NO2/c1-3-8(2)12(14)15-11-6-9-4-5-10(7-11)13-9/h3,9-11,13H,4-7H2,1

KLFGVBUPYUSQKV-YBULNHEOSA-N

C12H19NO2

CC=C(C)C(=O)OC1CC2CCC(C1)N2

209.28

Physical Properties

Property code	Value	Unit	Source
gf	65.21	kJ/mol	Joback Method
hf	-277.63	kJ/mol	Joback Method
hfus	31.25	kJ/mol	Joback Method
hvap	58.12	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	1.779		Crippen Method
mcvol	171.340	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1584.00		NIST Webbook
tb	620.19	K	Joback Method
tc	843.33	K	Joback Method
tf	407.75	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.99	J/mol×K	620.19	Joback Method
cpg	489.95	J/mol×K	657.38	Joback Method
cpg	507.71	J/mol×K	694.57	Joback Method
cpg	524.33	J/mol×K	731.76	Joback Method
cpg	539.88	J/mol×K	768.95	Joback Method
cpg	554.41	J/mol×K	806.14	Joback Method
cpg	567.98	J/mol×K	843.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R421700&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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