Propyl angelate

Other names:	propyl 2-methylisocrotonate
Inchi:	InChI=1S/C8H14O2/c1-4-6-10-8(9)7(3)5-2/h5H,4,6H2,1-3H3/b7-5-
InchiKey:	RZWMDOQSXWAAMC-ALCCZGGFSA-N
Formula:	C8H14O2
SMILES:	CC=C(C)C(=O)OCCC
Mol. weight [g/mol]:	142.20
CAS:	53082-57-8

Physical Properties

Property code	Value	Unit	Source
gf	-145.77	kJ/mol	Joback Method
hf	-345.82	kJ/mol	Joback Method
hfus	18.16	kJ/mol	Joback Method
hvap	42.60	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.906		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
rinpol	980.00		NIST Webbook
rinpol	994.30		NIST Webbook
rinpol	980.00		NIST Webbook
tb	462.77	K	Joback Method
tc	649.52	K	Joback Method
tf	233.04	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.21	J/mol×K	462.77	Joback Method
cpg	275.29	J/mol×K	493.90	Joback Method
cpg	286.87	J/mol×K	525.02	Joback Method
cpg	297.94	J/mol×K	556.15	Joback Method
cpg	308.52	J/mol×K	587.27	Joback Method

cpg	318.63	J/mol×K	618.40	Joback Method
cpg	328.27	J/mol×K	649.52	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=C53082578&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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