Pentyl (E)-2-methylbut-2-enoate

Other names:	Amyl tiglate
	Pentyl tiglate
Inchi:	InChI=1S/C10H18O2/c1-4-6-7-8-12-10(11)9(3)5-2/h5H,4,6-8H2,1-3H3/b9-5+
InchiKey:	XJWDRSSGOHXOLQ-WEVVVXLNSA-N
Formula:	C10H18O2
SMILES:	CC=C(C)C(=O)OCCCCC
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
gf	-128.93	kJ/mol	Joback Method
hf	-387.10	kJ/mol	Joback Method
hfus	23.34	kJ/mol	Joback Method
hvap	47.05	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.686		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	1174.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1174.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1519.00		NIST Webbook
tb	508.53	K	Joback Method
tc	691.44	K	Joback Method
tf	255.58	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	350.59	J/mol×K	508.53	Joback Method
cpg	364.62	J/mol×K	539.01	Joback Method
cpg	378.03	J/mol×K	569.50	Joback Method
cpg	390.86	J/mol×K	599.98	Joback Method
cpg	403.11	J/mol×K	630.47	Joback Method
cpg	414.81	J/mol×K	660.95	Joback Method
cpg	425.96	J/mol×K	691.44	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=U373726&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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