

2-Propenoic acid, 2-methyl-, pentyl ester

Other names:	amyl methacrylate methacrylic acid, pentyl ester pentyl 2-methyl-2-propenoate pentyl methacrylate
Inchi:	InChI=1S/C9H16O2/c1-4-5-6-7-11-9(10)8(2)3/h2,4-7H2,1,3H3
InchiKey:	GYDSPAVLTMAXHT-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	C=C(C)C(=O)OCCCC
Mol. weight [g/mol]:	156.22
CAS:	2849-98-1

Physical Properties

Property code	Value	Unit	Source
gf	-129.73	kJ/mol	Joback Method
hf	-358.25	kJ/mol	Joback Method
hfus	19.26	kJ/mol	Joback Method
hvap	44.19	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1064.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1062.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1328.00		NIST Webbook
ripol	1314.00		NIST Webbook
tb	478.17	K	Joback Method
tc	658.40	K	Joback Method
tf	247.63	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.67	J/mol×K	628.36	Joback Method
cpg	305.33	J/mol×K	478.17	Joback Method
cpg	318.20	J/mol×K	508.21	Joback Method
cpg	330.57	J/mol×K	538.25	Joback Method
cpg	342.43	J/mol×K	568.28	Joback Method
cpg	353.79	J/mol×K	598.32	Joback Method
cpg	375.07	J/mol×K	658.40	Joback Method
hvapt	47.60	kJ/mol	397.50	NIST Webbook

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=C2849981&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
High-Pressure Phase Behavior for Pentyl Acrylate and Pentyl Methacrylate in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je060122s

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
hvapt:	Enthalpy of vaporization at a given temperature
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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