2-Butenoic acid, 2-methyl-, pentyl ester, (Z)-

Other names: pentyl 2-methylisocrotonate
(Z)-Pentyl 2-methylbut-2-enoate
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-UITAMQMPSA-N
Formula: C10H18O2
SMILES: CC=C(C)C(=O)OCCCCC
Mol. weight [g/mol]: 170.25
CAS: 7785-63-9

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	1189.80		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=C7785639&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