4-Pentenoic 2-methylpropyl ester

Inchi: InChI=1S/C9H16O2/c1-4-5-6-9(10)11-7-8(2)3/h4,8H,1,5-7H2,2-3H3
InchiKey: PODLXXLZBYRGJW-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: C=CCCC(=O)OCC(C)C
Mol. weight [g/mol]: 156.22
CAS: 62030-45-9

Physical Properties

Property code	Value	Unit	Source
chl	-5340.00 ± 3.30	kJ/mol	NIST Webbook
gf	-123.62	kJ/mol	Joback Method
hf	-437.00 ± 4.00	kJ/mol	NIST Webbook
hfl	-488.00 ± 3.00	kJ/mol	NIST Webbook
hfus	17.05	kJ/mol	Joback Method
hvap	51.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-2.06		Crippen Method
logp	2.152		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
tb	477.85	K	Joback Method
tc	658.67	K	Joback Method
tf	246.59	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.61	J/mol×K	477.85	Joback Method
cpg	318.63	J/mol×K	507.99	Joback Method
cpg	331.13	J/mol×K	538.12	Joback Method
cpg	343.12	J/mol×K	568.26	Joback Method
cpg	354.60	J/mol×K	598.39	Joback Method
cpg	365.59	J/mol×K	628.53	Joback Method
cpg	376.08	J/mol×K	658.67	Joback Method

dvisc	0.0043503	Pa×s	246.59	Joback Method
dvisc	0.0019129	Pa×s	285.13	Joback Method
dvisc	0.0010229	Pa×s	323.68	Joback Method
dvisc	0.0006250	Pa×s	362.22	Joback Method
dvisc	0.0004198	Pa×s	400.76	Joback Method
dvisc	0.0003024	Pa×s	439.31	Joback Method
dvisc	0.0002296	Pa×s	477.85	Joback Method
hvapt	41.00	kJ/mol	293.00	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=C62030459&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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