PROPANOIC ACID, 2-METHYL-, 3-METHYL-2-BUTENYL ESTER

Other names: 3-methylbut-2-enyl isobutyrate
Prenyl isobutyrate
Inchi: InChI=1S/C9H16O2/c1-7(2)5-6-11-9(10)8(3)4/h5,8H,6H2,1-4H3
InchiKey: YSJHMPXIMIOXGU-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CC(C)=CCOC(=O)C(C)C
Mol. weight [g/mol]: 156.23

Physical Properties

Property code	Value	Unit	Source
af	0.4378		Cheméo Relay (1.0)
hf	-446.69	kJ/mol	Cheméo Relay (1.0)
hfus	17.22	kJ/mol	Joback Method
hvap	50.69	kJ/mol	Cheméo Relay (1.0)
ie	8.91	eV	Cheméo Relay (1.0)
logp	2.152		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	1053.00		NIST Webbook
rinpol	1053.00		NIST Webbook
tb	437.54	K	Cheméo Relay (1.0)
tc	619.53	K	Cheméo Relay (1.0)
tf	221.15	K	Cheméo Relay (1.0)
vc	0.518	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.09	J/mol×K	485.21	Joback Method
cpg	319.56	J/mol×K	516.68	Joback Method
cpg	332.44	J/mol×K	548.16	Joback Method
cpg	344.74	J/mol×K	579.63	Joback Method
cpg	356.48	J/mol×K	611.11	Joback Method
cpg	367.66	J/mol×K	642.58	Joback Method

cpg	378.31	J/mol×K	674.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76649235&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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