Isovaleric acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C11H22O3/c1-9(2)7-11(12)14-8-10(3)5-6-13-4/h9-10H,5-8H2,1-4H3
InchiKey: JJUFYIUMRUMHLH-UHFFFAOYSA-N
Formula: C11H22O3
SMILES: COCCC(C)COC(=O)CC(C)C
Mol. weight [g/mol]: 202.29

Physical Properties

Property code	Value	Unit	Source
gf	-302.06	kJ/mol	Joback Method
hf	-657.95	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	50.87	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	2.248		Crippen Method
mcvol	179.160	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	1313.00		NIST Webbook
rinpol	1313.00		NIST Webbook
tb	548.91	K	Joback Method
tc	725.84	K	Joback Method
tf	278.12	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.83	J/mol×K	548.91	Joback Method
cpg	458.24	J/mol×K	578.40	Joback Method
cpg	473.06	J/mol×K	607.89	Joback Method
cpg	487.29	J/mol×K	637.38	Joback Method
cpg	500.93	J/mol×K	666.86	Joback Method
cpg	513.98	J/mol×K	696.35	Joback Method
cpg	526.44	J/mol×K	725.84	Joback Method
dvisc	0.0043534	Pa×s	278.12	Joback Method

dvisc	0.0016670	Pa×s	323.25	Joback Method
dvisc	0.0008076	Pa×s	368.38	Joback Method
dvisc	0.0004583	Pa×s	413.52	Joback Method
dvisc	0.0002908	Pa×s	458.65	Joback Method
dvisc	0.0002001	Pa×s	503.78	Joback Method
dvisc	0.0001465	Pa×s	548.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360653&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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