Isobutyric acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C10H20O3/c1-8(2)10(11)13-7-9(3)5-6-12-4/h8-9H,5-7H2,1-4H3
InchiKey: WYQRCEYZRBWUHU-UHFFFAOYSA-N
Formula: C10H20O3
SMILES: COCCC(C)COC(=O)C(C)C
Mol. weight [g/mol]: 188.26

Physical Properties

Property code	Value	Unit	Source
gf	-310.48	kJ/mol	Joback Method
hf	-637.31	kJ/mol	Joback Method
hfus	18.59	kJ/mol	Joback Method
hvap	48.64	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.858		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1229.00		NIST Webbook
rinpol	1229.00		NIST Webbook
tb	526.03	K	Joback Method
tc	704.59	K	Joback Method
tf	266.85	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.72	J/mol×K	526.03	Joback Method
cpg	462.43	J/mol×K	674.83	Joback Method
cpg	449.98	J/mol×K	645.07	Joback Method
cpg	436.98	J/mol×K	615.31	Joback Method
cpg	423.43	J/mol×K	585.55	Joback Method
cpg	409.35	J/mol×K	555.79	Joback Method
cpg	474.34	J/mol×K	704.59	Joback Method
dvisc	0.0001618	Pa×s	526.03	Joback Method

dvisc	0.0002205	Pa×s	482.83	Joback Method
dvisc	0.0003192	Pa×s	439.64	Joback Method
dvisc	0.0005009	Pa×s	396.44	Joback Method
dvisc	0.0008775	Pa×s	353.24	Joback Method
dvisc	0.0017975	Pa×s	310.05	Joback Method
dvisc	0.0046442	Pa×s	266.85	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=U354635&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
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