

Formic acid, 2-(2-methoxyethyl)hexyl ester

Inchi: InChI=1S/C10H20O3/c1-3-4-5-10(6-7-12-2)8-13-9-11/h9-10H,3-8H2,1-2H3
InchiKey: SJUJLXBXNWZKAQ-UHFFFAOYSA-N
Formula: C10H20O3
SMILES: CCCCC(CCOC)COC=O
Mol. weight [g/mol]: 188.26

Physical Properties

Property code	Value	Unit	Source
gf	-278.64	kJ/mol	Joback Method
hf	-605.03	kJ/mol	Joback Method
hfus	22.80	kJ/mol	Joback Method
hvap	49.01	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	2.002		Crippen Method
mvol	165.070	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
rinpol	1288.00		NIST Webbook
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tb	521.26	K	Joback Method
tc	692.43	K	Joback Method
tf	273.92	K	Joback Method
vc	0.642	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.00	J/molxK	521.26	Joback Method
cpg	408.94	J/molxK	549.79	Joback Method
cpg	422.39	J/molxK	578.32	Joback Method
cpg	435.35	J/molxK	606.85	Joback Method
cpg	447.82	J/molxK	635.37	Joback Method
cpg	459.79	J/molxK	663.90	Joback Method
cpg	471.28	J/molxK	692.43	Joback Method
dvisc	0.0037329	Paxs	273.92	Joback Method

dvisc	0.0016366	Paxs	315.14	Joback Method
dvisc	0.0008683	Paxs	356.37	Joback Method
dvisc	0.0005254	Paxs	397.59	Joback Method
dvisc	0.0003494	Paxs	438.81	Joback Method
dvisc	0.0002492	Paxs	480.04	Joback Method
dvisc	0.0001875	Paxs	521.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U367907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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