ethyl 2-methylbutanoate-d-3

Inchi: InChI=1S/C7H14O2/c1-4-6(3)7(8)9-5-2/h6H,4-5H2,1-3H3/i1D3
InchiKey: HCRBXQFHJMCTLF-FIBGUPNXSA-N
Formula: C7H11D3O2
SMILES: CCOC(=O)C(C)CC
Mol. weight [g/mol]: 133.20

Physical Properties

Property code	Value	Unit	Source
gf	-228.30	kJ/mol	Joback Method
hf	-437.89	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	39.94	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.596		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
ripol	1053.00		NIST Webbook
tb	435.41	K	Joback Method
tc	615.76	K	Joback Method
tf	225.81	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.73	J/mol×K	435.41	Joback Method
cpg	250.17	J/mol×K	465.47	Joback Method
cpg	261.22	J/mol×K	495.53	Joback Method
cpg	271.87	J/mol×K	525.58	Joback Method
cpg	282.12	J/mol×K	555.64	Joback Method
cpg	291.98	J/mol×K	585.70	Joback Method
cpg	301.45	J/mol×K	615.76	Joback Method
dvisc	0.0047724	Pa×s	225.81	Joback Method
dvisc	0.0021099	Pa×s	260.74	Joback Method

dvisc	0.0011312	Pa×s	295.68	Joback Method
dvisc	0.0006919	Pa×s	330.61	Joback Method
dvisc	0.0004649	Pa×s	365.54	Joback Method
dvisc	0.0003348	Pa×s	400.48	Joback Method
dvisc	0.0002542	Pa×s	435.41	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R322673&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume