propyl butanoate-d3

Inchi: InChI=1S/C7H14O2/c1-3-5-7(8)9-6-4-2/h3-6H2,1-2H3/i1D3
InchiKey: HUAZGNHGCJGYNP-FIBGUPNXSA-N
Formula: C7H11D3O2
SMILES: CCCOC(=O)CCC
Mol. weight [g/mol]: 133.20

Physical Properties

Property code	Value	Unit	Source
gf	-225.86	kJ/mol	Joback Method
hf	-432.61	kJ/mol	Joback Method
hfus	16.67	kJ/mol	Joback Method
hvap	40.33	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.740		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
ripol	1122.00		NIST Webbook
ripol	1122.00		NIST Webbook
tb	435.85	K	Joback Method
tc	612.24	K	Joback Method
tf	240.81	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.65	J/mol×K	435.85	Joback Method
cpg	290.48	J/mol×K	582.84	Joback Method
cpg	280.85	J/mol×K	553.44	Joback Method
cpg	270.86	J/mol×K	524.04	Joback Method
cpg	260.50	J/mol×K	494.65	Joback Method
cpg	249.76	J/mol×K	465.25	Joback Method
cpg	299.73	J/mol×K	612.24	Joback Method
dvisc	0.0002656	Pa×s	435.85	Joback Method

dvisc	0.0003401	Pa×s	403.34	Joback Method
dvisc	0.0004549	Pa×s	370.84	Joback Method
dvisc	0.0006434	Pa×s	338.33	Joback Method
dvisc	0.0009795	Pa×s	305.82	Joback Method
dvisc	0.0016480	Pa×s	273.32	Joback Method
dvisc	0.0031909	Pa×s	240.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R329154&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume