n-Butyric acid tetrahydrofurfuryl ester

Other names:	2-Furanmethanol, tetrahydro-, propanoate
	2-Furanemethanol, tetrahydro-, propanoate
	Tetrahydrofurfuryl alcohol propionate
	Tetrahydrofurfuryl propionate
Inchi:	InChI=1S/C8H14O3/c1-2-8(9)11-6-7-4-3-5-10-7/h7H,2-6H2,1H3
InchiKey:	FMKCDSXOYLTWBR-UHFFFAOYSA-N
Formula:	C8H14O3
SMILES:	CCC(=O)OCC1CCCO1
Mol. weight [g/mol]:	158.19
CAS:	637-65-0

Physical Properties

Property code	Value	Unit	Source
gf	-267.01	kJ/mol	Joback Method
hf	-524.77	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	47.33	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.119		Crippen Method
mcvol	126.030	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	1153.00		NIST Webbook
ripol	1632.00		NIST Webbook
tb	478.70	K	NIST Webbook
tc	703.64	K	Joback Method
tf	289.55	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.97	J/mol×K	500.96	Joback Method
cpg	308.60	J/mol×K	534.74	Joback Method
cpg	322.51	J/mol×K	568.52	Joback Method

cpg	335.72	J/mol×K	602.30	Joback Method
cpg	348.23	J/mol×K	636.08	Joback Method
cpg	360.07	J/mol×K	669.86	Joback Method
cpg	371.24	J/mol×K	703.64	Joback Method
dvisc	0.0034626	Pa×s	289.55	Joback Method
dvisc	0.0019229	Pa×s	324.79	Joback Method
dvisc	0.0011982	Pa×s	360.02	Joback Method
dvisc	0.0008123	Pa×s	395.25	Joback Method
dvisc	0.0005869	Pa×s	430.49	Joback Method
dvisc	0.0004454	Pa×s	465.72	Joback Method
dvisc	0.0003514	Pa×s	500.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.20	K	0.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C637650&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

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