1,4-Butanediol, monoacetate

Inchi: InChI=1S/C6H12O3/c1-6(8)9-5-3-2-4-7/h7H,2-5H2,1H3
InchiKey: FLVQOAUAIBIIGO-UHFFFAOYSA-N
Formula: C6H12O3
SMILES: CC(=O)OCCCCO
Mol. weight [g/mol]: 132.16

Physical Properties

Property code	Value	Unit	Source
gf	-371.10	kJ/mol	Joback Method
hf	-564.20	kJ/mol	Joback Method
hfus	18.17	kJ/mol	Joback Method
hvap	54.78	kJ/mol	Joback Method
log10ws	-0.46		Crippen Method
logp	0.322		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
ripol	1826.00		NIST Webbook
ripol	1826.00		NIST Webbook
tb	505.15	K	Joback Method
tc	676.09	K	Joback Method
tf	290.36	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.47	J/mol×K	505.15	Joback Method
cpg	286.56	J/mol×K	647.60	Joback Method
cpg	278.97	J/mol×K	619.11	Joback Method
cpg	271.06	J/mol×K	590.62	Joback Method
cpg	262.85	J/mol×K	562.13	Joback Method
cpg	254.32	J/mol×K	533.64	Joback Method
cpg	293.84	J/mol×K	676.09	Joback Method
dvisc	0.0001569	Pa×s	505.15	Joback Method

dvisc	0.0002454	Pa×s	469.35	Joback Method
dvisc	0.0004134	Pa×s	433.55	Joback Method
dvisc	0.0007647	Pa×s	397.75	Joback Method
dvisc	0.0015977	Pa×s	361.96	Joback Method
dvisc	0.0039241	Pa×s	326.16	Joback Method
dvisc	0.0120283	Pa×s	290.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410438&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume