Propionaldehyde, dipropargal acetal

Inchi: InChI=1S/C9H12O2/c1-4-7-10-9(6-3)11-8-5-2/h1-2,9H,6-8H2,3H3
InchiKey: SPAJYYACTLORPH-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: C#CCOC(CC)OCC#C
Mol. weight [g/mol]: 152.19
CAS: 4033-07-2

Physical Properties

Property code	Value	Unit	Source
gf	258.60	kJ/mol	Joback Method
hf	84.99	kJ/mol	Joback Method
hfus	23.87	kJ/mol	Joback Method
hvap	39.78	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.022		Crippen Method
mcvol	132.210	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
tb	429.96	K	Joback Method
tc	620.71	K	Joback Method
tf	314.59	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.92	J/mol×K	429.96	Joback Method
cpg	277.08	J/mol×K	461.75	Joback Method
cpg	287.82	J/mol×K	493.54	Joback Method
cpg	298.14	J/mol×K	525.33	Joback Method
cpg	308.06	J/mol×K	557.13	Joback Method
cpg	317.56	J/mol×K	588.92	Joback Method
cpg	326.67	J/mol×K	620.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4033072&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume