Benzene, 1-(1-formylethyl)-4-(1-buten-3-yl)-

Inchi: InChI=1S/C13H16O/c1-4-10(2)12-5-7-13(8-6-12)11(3)9-14/h4-11H,1H2,2-3H3
InchiKey: DRNYGFDTUBEIAL-UHFFFAOYSA-N
Formula: C13H16O
SMILES: C=CC(C)c1ccc(C(C)C=O)cc1
Mol. weight [g/mol]: 188.27

Physical Properties

Property code	Value	Unit	Source
gf	144.80	kJ/mol	Joback Method
hf	-57.30	kJ/mol	Joback Method
hfus	17.04	kJ/mol	Joback Method
hvap	52.74	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.278		Crippen Method
mcvol	167.540	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
tb	572.96	K	Joback Method
tc	787.03	K	Joback Method
tf	285.45	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.60	J/mol×K	572.96	Joback Method
cpg	467.04	J/mol×K	751.35	Joback Method
cpg	454.92	J/mol×K	715.67	Joback Method
cpg	441.95	J/mol×K	680.00	Joback Method
cpg	428.11	J/mol×K	644.32	Joback Method
cpg	413.34	J/mol×K	608.64	Joback Method
cpg	478.36	J/mol×K	787.03	Joback Method
dvisc	0.0002025	Pa×s	572.96	Joback Method

dvisc	0.0002664	Pa×s	525.04	Joback Method
dvisc	0.0003701	Pa×s	477.12	Joback Method
dvisc	0.0005535	Pa×s	429.21	Joback Method
dvisc	0.0009159	Pa×s	381.29	Joback Method
dvisc	0.0017515	Pa×s	333.37	Joback Method
dvisc	0.0041640	Pa×s	285.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U161466&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume