«alpha»-Butylcinnamic aldehyde

Other names: «alpha»-butylcinnamaldehyde
Inchi: InChI=1S/C13H16O/c1-2-3-7-13(11-14)10-12-8-5-4-6-9-12/h4-6,8-11H,2-3,7H2,1H3/b13-
InchiKey: GFBCBQNBXRPRQD-JLHYYAGUSA-N
Formula: C13H16O
SMILES: CCCCC(C=O)=Cc1ccccc1
Mol. weight [g/mol]: 188.27
CAS: 7492-44-6

Physical Properties

Property code	Value	Unit	Source
gf	143.14	kJ/mol	Joback Method
hf	-53.27	kJ/mol	Joback Method
hfus	24.65	kJ/mol	Joback Method
hvap	53.57	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.459		Crippen Method
mcvol	167.540	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
rinpol	1535.00		NIST Webbook
rinpol	1535.00		NIST Webbook
ripol	2160.00		NIST Webbook
ripol	2160.00		NIST Webbook
tb	576.22	K	Joback Method
tc	788.88	K	Joback Method
tf	285.65	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.65	J/mol×K	576.22	Joback Method
cpg	413.25	J/mol×K	611.66	Joback Method
cpg	427.86	J/mol×K	647.11	Joback Method
cpg	441.53	J/mol×K	682.55	Joback Method

cpg	454.31	J/mol×K	717.99	Joback Method
cpg	466.27	J/mol×K	753.44	Joback Method
cpg	477.46	J/mol×K	788.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7492446&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume