n-Butyl cinnamate

Other names:	2-Propenoic acid, 3-phenyl-, butyl ester
	Butyl cinnamate
	Cinnamic acid butyl ester
	Cinnamic acid n-butyl ester
	Eliminoxy
	n-Butyl phenylacrylate
	Cinnamate de n-butyle
	Butyl 3-phenyl-2-propenoate
	NSC 71966
Inchi:	InChI=1S/C13H16O2/c1-2-3-11-15-13(14)10-9-12-7-5-4-6-8-12/h4-10H,2-3,11H2,1H3/b1
InchiKey:	OHHIVLJVBNCSHV-MDZDMXLPSA-N
Formula:	C13H16O2
SMILES:	CCCCOC(=O)C=Cc1ccccc1
Mol. weight [g/mol]:	204.26
CAS:	538-65-8

Physical Properties

Property code	Value	Unit	Source
gf	17.29	kJ/mol	Joback Method
hf	-202.70	kJ/mol	Joback Method
hfus	26.46	kJ/mol	Joback Method
hvap	55.92	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.043		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
tb	603.97	K	Joback Method
tc	815.36	K	Joback Method
tf	329.77	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	423.08	J/mol×K	603.97	Joback Method
cpg	490.65	J/mol×K	780.13	Joback Method
cpg	478.84	J/mol×K	744.90	Joback Method
cpg	466.22	J/mol×K	709.66	Joback Method
cpg	452.75	J/mol×K	674.43	Joback Method
cpg	438.38	J/mol×K	639.20	Joback Method
cpg	501.68	J/mol×K	815.36	Joback Method
dvisc	0.0001434	Pa×s	603.97	Joback Method
dvisc	0.0001858	Pa×s	558.27	Joback Method
dvisc	0.0002522	Pa×s	512.57	Joback Method
dvisc	0.0003633	Pa×s	466.87	Joback Method
dvisc	0.0005667	Pa×s	421.17	Joback Method
dvisc	0.0009848	Pa×s	375.47	Joback Method
dvisc	0.0019948	Pa×s	329.77	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C538658&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume