.beta.-Phenethyl butyrate

Other names:	2-Phenethyl butanoate
	2-phenylethyl butanoate
	2-phenylethyl butyrate
	Benzylcarbinyl butyrate
	Butanoic acid, 2-phenylethyl ester
	Butyric acid, phenethyl ester
	Phenethyl butanoate
	Phenylethyl butyrate
	phenethyl butyrate
	«beta»-Phenethyl n-butanoate
	«beta»-Phenylethyl n-butyrate
Inchi:	InChI=1S/C12H16O2/c1-2-6-12(13)14-10-9-11-7-4-3-5-8-11/h3-5,7-8H,2,6,9-10H2,1H3
InchiKey:	WFNDDSQUKATKNX-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	192.26

Physical Properties

Property code	Value	Unit	Source
af	0.5820		Cheméo Relay (1.0)
gf	-71.35	kJ/mol	Joback Method
hf	-354.13	kJ/mol	Cheméo Relay (1.0)
hfus	23.66	kJ/mol	Joback Method
hvap	69.92	kJ/mol	Cheméo Relay (1.0)
ie	8.71	eV	Cheméo Relay (1.0)
log10ws	-2.87		Cheméo Relay (1.0)
logp	2.572		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
tb	530.27	K	Cheméo Relay (1.0)
tc	732.68	K	Cheméo Relay (1.0)
tf	224.02	K	Cheméo Relay (1.0)
vc	0.609	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.04	J/mol×K	576.93	Joback Method
cpg	472.86	J/mol×K	782.93	Joback Method
cpg	461.69	J/mol×K	748.60	Joback Method
cpg	449.76	J/mol×K	714.26	Joback Method
cpg	437.06	J/mol×K	679.93	Joback Method
cpg	423.55	J/mol×K	645.60	Joback Method
cpg	409.22	J/mol×K	611.26	Joback Method
dvisc	0.0004524	Pa×s	450.25	Joback Method
dvisc	0.0001842	Pa×s	576.93	Joback Method
dvisc	0.0002371	Pa×s	534.70	Joback Method
dvisc	0.0003185	Pa×s	492.48	Joback Method
dvisc	0.0022442	Pa×s	323.58	Joback Method
dvisc	0.0006908	Pa×s	408.03	Joback Method
dvisc	0.0011633	Pa×s	365.81	Joback Method
hvapt	69.70	kJ/mol	298.15	Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103526&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Vapor pressures and vaporization enthalpies of a series of esters used in flavors by correlation gas chromatography:	https://www.doi.org/10.1016/j.jct.2015.02.015

Legend

af:	Acentric Factor
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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