Benzenepropanoic acid, phenylmethyl ester

Other names:	Benzyl hydrocinnamic acid
	3-Phenylpropionic acid, benzyl ester
	Benzyl hydrocinnamate
	Benzyl 3-phenylpropanoate
Inchi:	InChI=1S/C16H16O2/c17-16(12-11-14-7-3-1-4-8-14)18-13-15-9-5-2-6-10-15/h1-10H,11-1
InchiKey:	IGUMLGLEYCGKBJ-UHFFFAOYSA-N
Formula:	C16H16O2
SMILES:	O=C(CCc1ccccc1)OCc1ccccc1
Mol. weight [g/mol]:	240.30
CAS:	22767-96-0

Physical Properties

Property code	Value	Unit	Source
gf	74.74	kJ/mol	Joback Method
hf	-145.31	kJ/mol	Joback Method
hfus	28.07	kJ/mol	Joback Method
hvap	64.92	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.363		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	1941.70		NIST Webbook
rinpol	1941.70		NIST Webbook
tb	695.13	K	Joback Method
tc	928.08	K	Joback Method
tf	395.08	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.86	J/mol×K	695.13	Joback Method
cpg	587.75	J/mol×K	889.25	Joback Method
cpg	576.23	J/mol×K	850.43	Joback Method

cpg	563.64	J/mol×K	811.60	Joback Method
cpg	549.92	J/mol×K	772.78	Joback Method
cpg	535.01	J/mol×K	733.95	Joback Method
cpg	598.26	J/mol×K	928.08	Joback Method
dvisc	0.0001223	Pa×s	695.13	Joback Method
dvisc	0.0001572	Pa×s	645.12	Joback Method
dvisc	0.0002108	Pa×s	595.11	Joback Method
dvisc	0.0002983	Pa×s	545.11	Joback Method
dvisc	0.0004527	Pa×s	495.10	Joback Method
dvisc	0.0007547	Pa×s	445.09	Joback Method
dvisc	0.0014320	Pa×s	395.08	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22767960&Units=SI

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