.alpha.-Cyanobenzyl benzoate

Other names:	Mandelonitrile, benzoate (ester)
	«alpha»-Cyanobenzyl benzoate
	Mandelonitrile benzoate
	Benzoic acid, alpha-cyanobenzyl ester
Inchi:	InChI=1S/C15H11NO2/c16-11-14(12-7-3-1-4-8-12)18-15(17)13-9-5-2-6-10-13/h1-10,14H
InchiKey:	AXAACNNFMJZAGJ-UHFFFAOYSA-N
Formula:	C15H11NO2
SMILES:	N#CC(OC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	237.26

Physical Properties

Property code	Value	Unit	Source
af	0.6060		Cheméo Relay (1.0)
hf	-8.69	kJ/mol	Cheméo Relay (1.0)
hfus	23.46	kJ/mol	Joback Method
hvap	96.11	kJ/mol	Cheméo Relay (1.0)
ie	9.42	eV	Cheméo Relay (1.0)
log10ws	-4.10		Cheméo Relay (1.0)
logp	3.108		Crippen Method
mcvol	183.510	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
tb	582.58	K	Cheméo Relay (1.0)
tc	883.38	K	Cheméo Relay (1.0)
tf	365.18	K	Cheméo Relay (1.0)
vc	0.659	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.71	J/mol×K	773.89	Joback Method
cpg	500.02	J/mol×K	816.03	Joback Method
cpg	511.14	J/mol×K	858.16	Joback Method
cpg	521.13	J/mol×K	900.30	Joback Method
cpg	530.07	J/mol×K	942.44	Joback Method

cpg	538.01	J/mol×K	984.58	Joback Method
cpg	545.02	J/mol×K	1026.71	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4242460&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):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
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