Benzeneacetonitrile, «alpha»-(benzoyloxy)-

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]:	237.25
CAS:	4242-46-0

Physical Properties

Property code	Value	Unit	Source
gf	197.06	kJ/mol	Joback Method
hf	34.93	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	72.78	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.108		Crippen Method
mcvol	183.510	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
tb	773.89	K	Joback Method
tc	1026.71	K	Joback Method
tf	433.80	K	Joback Method
vc	0.704	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4242460&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume