Benzoyl fluoride

Inchi: InChI=1S/C7H5FO/c8-7(9)6-4-2-1-3-5-6/h1-5H
InchiKey: HPMLGNIUXVXALD-UHFFFAOYSA-N
Formula: C7H5FO
SMILES: O=C(F)c1ccccc1
Mol. weight [g/mol]: 124.11
CAS: 455-32-3

Physical Properties

Property code	Value	Unit	Source
gf	-203.26	kJ/mol	Joback Method
hf	-259.97	kJ/mol	Joback Method
hfus	12.61	kJ/mol	Joback Method
hvap	39.38	kJ/mol	Joback Method
ie	10.60	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	9.78	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.67	eV	NIST Webbook
ie	10.60	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	1.796		Crippen Method
mcvol	89.070	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
tb	433.00	K	NIST Webbook
tb	433.20	K	NIST Webbook
tb	433.00 ± 1.00	K	NIST Webbook
tc	652.05	K	Joback Method
tf	245.59	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	161.63	J/mol×K	439.38	Joback Method
cpg	171.55	J/mol×K	474.82	Joback Method
cpg	180.84	J/mol×K	510.27	Joback Method
cpg	189.53	J/mol×K	545.71	Joback Method
cpg	197.63	J/mol×K	581.16	Joback Method
cpg	205.17	J/mol×K	616.60	Joback Method
cpg	212.18	J/mol×K	652.05	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=C455323&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
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
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