2-Propyn-1-ol, benzoate

Other names: 2-propynyl benzoate
Inchi: InChI=1S/C10H8O2/c1-2-8-12-10(11)9-6-4-3-5-7-9/h1,3-7H,8H2
InchiKey: NBDHEMWCIUHARG-UHFFFAOYSA-N
Formula: C10H8O2
SMILES: C#CCOC(=O)c1ccccc1
Mol. weight [g/mol]: 160.17
CAS: 6750-04-5

Physical Properties

Property code	Value	Unit	Source
gf	134.88	kJ/mol	Joback Method
hf	33.90	kJ/mol	Joback Method
hfus	21.46	kJ/mol	Joback Method
hvap	49.14	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.477		Crippen Method
mcvol	126.840	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
rinpol	1262.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1252.00		NIST Webbook
ripol	2003.00		NIST Webbook
ripol	2004.00		NIST Webbook
ripol	1998.00		NIST Webbook
ripol	2003.00		NIST Webbook
ripol	2004.00		NIST Webbook

ripol	2017.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	1981.00		NIST Webbook
ripol	2026.00		NIST Webbook
tb	521.29	K	Joback Method
tc	749.90	K	Joback Method
tf	348.01	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.07	J/mol×K	521.29	Joback Method
cpg	277.09	J/mol×K	559.39	Joback Method
cpg	288.33	J/mol×K	597.49	Joback Method
cpg	298.81	J/mol×K	635.60	Joback Method
cpg	308.56	J/mol×K	673.70	Joback Method
cpg	317.62	J/mol×K	711.80	Joback Method
cpg	326.00	J/mol×K	749.90	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=C6750045&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume