

Ethanone, 2-(benzoyloxy)-1,2-diphenyl-

Other names:	Desyl benzoate
Inchi:	InChI=1S/C21H16O3/c22-19(16-10-4-1-5-11-16)20(17-12-6-2-7-13-17)24-21(23)18-14-8
InchiKey:	FGOSBCXOMBLILW-UHFFFAOYSA-N
Formula:	C21H16O3
SMILES:	O=C(OC(C(=O)c1ccccc1)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	316.35
CAS:	1459-20-7

Physical Properties

Property code	Value	Unit	Source
gf	97.89	kJ/mol	Joback Method
hf	-129.84	kJ/mol	Joback Method
hfus	33.13	kJ/mol	Joback Method
hvap	84.68	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.468		Crippen Method
mcvol	244.480	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
tb	889.64	K	Joback Method
tc	1149.72	K	Joback Method
tf	512.78	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.24	J/mol×K	889.64	Joback Method
cpg	766.22	J/mol×K	1106.37	Joback Method
cpg	758.09	J/mol×K	1063.02	Joback Method
cpg	748.84	J/mol×K	1019.68	Joback Method
cpg	738.36	J/mol×K	976.33	Joback Method
cpg	726.53	J/mol×K	932.99	Joback Method
cpg	773.37	J/mol×K	1149.72	Joback Method
dvisc	0.0000600	Pa×s	889.64	Joback Method

dvisc	0.0000778	Pa×s	826.83	Joback Method
dvisc	0.0001053	Pa×s	764.02	Joback Method
dvisc	0.0001504	Pa×s	701.21	Joback Method
dvisc	0.0002304	Pa×s	638.40	Joback Method
dvisc	0.0003874	Pa×s	575.59	Joback Method
dvisc	0.0007399	Pa×s	512.78	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=C1459207&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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