

(4-(4-Benzoyl-phenoxy)-phenyl)-phenyl-methanone

Inchi:	InChI=1S/C26H18O3/c27-25(19-7-3-1-4-8-19)21-11-15-23(16-12-21)29-24-17-13-22(14-
InchiKey:	RFESNAMUUSDBQQ-UHFFFAOYSA-N
Formula:	C26H18O3
SMILES:	O=C(c1ccccc1)c1ccc(Oc2ccc(C(=O)c3ccccc3)cc2)cc1
Mol. weight [g/mol]:	378.42
CAS:	6966-89-8

Physical Properties

Property code	Value	Unit	Source
gf	235.58	kJ/mol	Joback Method
hf	-14.17	kJ/mol	Joback Method
hfus	42.87	kJ/mol	Joback Method
hvap	99.80	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.941		Crippen Method
mcvol	291.170	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
tb	1041.12	K	Joback Method
tc	1313.92	K	Joback Method
tf	635.59	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.18	J/molxK	1041.12	Joback Method
cpg	899.05	J/molxK	1086.59	Joback Method
cpg	908.57	J/molxK	1132.05	Joback Method
cpg	916.88	J/molxK	1177.52	Joback Method
cpg	924.15	J/molxK	1222.99	Joback Method
cpg	930.54	J/molxK	1268.45	Joback Method
cpg	936.19	J/molxK	1313.92	Joback Method
dvisc	0.0002859	Paxs	635.59	Joback Method
dvisc	0.0001708	Paxs	703.18	Joback Method

dvisc	0.0001117	Paxs	770.77	Joback Method
dvisc	0.0000783	Paxs	838.36	Joback Method
dvisc	0.0000578	Paxs	905.94	Joback Method
dvisc	0.0000445	Paxs	973.53	Joback Method
dvisc	0.0000355	Paxs	1041.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6966898&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
mcvol:	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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