Resorcinol, 2,4-dibenzoyl-6-hexyl-

Inchi: InChI=1S/C26H26O4/c1-2-3-4-7-16-20-17-21(23(27)18-12-8-5-9-13-18)26(30)22(25(20)2
InchiKey: LGOMKSQEZOHEAQ-UHFFFAOYSA-N
Formula: C26H26O4
SMILES: CCCCCCc1cc(C(=O)c2ccccc2)c(O)c(C(=O)c2ccccc2)c1O
Mol. weight [g/mol]: 402.48

Physical Properties

Property code	Value	Unit	Source
gf	-81.07	kJ/mol	Joback Method
hf	-473.10	kJ/mol	Joback Method
hfus	59.20	kJ/mol	Joback Method
hvap	121.14	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	5.683		Crippen Method
mcvol	320.800	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
tb	1153.26	K	Joback Method
tc	1418.08	K	Joback Method
tf	810.38	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.84	J/mol×K	1153.26	Joback Method
cpg	1108.93	J/mol×K	1197.40	Joback Method
cpg	1129.94	J/mol×K	1241.53	Joback Method
cpg	1152.14	J/mol×K	1285.67	Joback Method
cpg	1175.85	J/mol×K	1329.81	Joback Method
cpg	1201.35	J/mol×K	1373.94	Joback Method
cpg	1228.94	J/mol×K	1418.08	Joback Method
dvisc	0.0000006	Pa×s	810.38	Joback Method
dvisc	0.0000003	Pa×s	867.53	Joback Method
dvisc	0.0000002	Pa×s	924.67	Joback Method

dvisc	9.6199859e-08	Pa×s	981.82	Joback Method
dvisc	6.0514769e-08	Pa×s	1038.97	Joback Method
dvisc	3.9952092e-08	Pa×s	1096.11	Joback Method
dvisc	2.7484535e-08	Pa×s	1153.26	Joback Method

Sources

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=B6000809&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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