

# trans-1,2-Bis(4-fluorobenzoyl)ethylene

<b>Inchi:</b>	InChI=1S/C16H10F2O2/c17-13-5-1-11(2-6-13)15(19)9-10-16(20)12-3-7-14(18)8-4-12/h1
<b>InchiKey:</b>	OXUZAAMYHTYRBZ-MDZDMLPSA-N
<b>Formula:</b>	C16H10F2O2
<b>SMILES:</b>	O=C(C=CC(=O)c1ccc(F)cc1)c1ccc(F)cc1
<b>Mol. weight [g/mol]:</b>	272.25
<b>CAS:</b>	25650-13-9

## Physical Properties

Property code	Value	Unit	Source
gf	-277.84	kJ/mol	Joback Method
hf	-423.61	kJ/mol	Joback Method
hfus	34.06	kJ/mol	Joback Method
hvap	68.90	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.587		Crippen Method
mvol	191.160	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
tb	739.24	K	Joback Method
tc	971.08	K	Joback Method
tf	443.92	K	Joback Method
vc	0.744	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.01	J/molxK	739.24	Joback Method
cpg	509.38	J/molxK	777.88	Joback Method
cpg	520.74	J/molxK	816.52	Joback Method
cpg	531.17	J/molxK	855.16	Joback Method
cpg	540.74	J/molxK	893.80	Joback Method
cpg	549.53	J/molxK	932.44	Joback Method
cpg	557.62	J/molxK	971.08	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C25650139&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25650139&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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