

3-[3-(Benzoyloxy)propoxy]propyl benzoate

Other names:	3,3'-oxydipropyl dibenzoate
Inchi:	InChI=1S/C20H22O5/c21-19(17-9-3-1-4-10-17)24-15-7-13-23-14-8-16-25-20(22)18-11-5
InchiKey:	BYQDGAVOOHIJQS-UHFFFAOYSA-N
Formula:	C20H22O5
SMILES:	O=C(OCCCCOCCOC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	342.39
CAS:	94-51-9

Physical Properties

Property code	Value	Unit	Source
gf	-230.50	kJ/mol	Joback Method
hf	-604.89	kJ/mol	Joback Method
hfus	42.40	kJ/mol	Joback Method
hvap	85.39	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.497		Crippen Method
mcvol	265.890	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
tb	885.36	K	Joback Method
tc	1107.59	K	Joback Method
tf	534.55	K	Joback Method
vc	1.006	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.91	J/molxK	885.36	Joback Method
cpg	864.66	J/molxK	1070.55	Joback Method
cpg	856.29	J/molxK	1033.51	Joback Method
cpg	846.66	J/molxK	996.48	Joback Method
cpg	835.74	J/molxK	959.44	Joback Method
cpg	823.50	J/molxK	922.40	Joback Method
cpg	871.79	J/molxK	1107.59	Joback Method
dvisc	0.0000414	Paxs	885.36	Joback Method

dvisc	0.0000532	Paxs	826.89	Joback Method
dvisc	0.0000709	Paxs	768.42	Joback Method
dvisc	0.0000990	Paxs	709.96	Joback Method
dvisc	0.0001468	Paxs	651.49	Joback Method
dvisc	0.0002354	Paxs	593.02	Joback Method
dvisc	0.0004184	Paxs	534.55	Joback Method

Sources

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=C94519&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ 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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