

1-{2-[2-(Diethylamino)ethoxy]phenyl}-3-phenylpropan-1-one

Other names:	1-Propanone, 1-[2-[2-(diethylamino)ethoxy]phenyl]-3-phenyl- 2'-[2-(Diethylamino)ethoxy]-3-phenylpropiophenone LG-11457
Inchi:	InChI=1S/C21H27NO2/c1-3-22(4-2)16-17-24-21-13-9-8-12-19(21)20(23)15-14-18-10-6-5
InchiKey:	OEGDFSLNGABBKJ-UHFFFAOYSA-N
Formula:	C21H27NO2
SMILES:	CCN(CC)CCOc1ccccc1C(=O)CCc1ccccc1
Mol. weight [g/mol]:	325.45

Physical Properties

Property code	Value	Unit	Source
hfus	43.65	kJ/mol	Joback Method
ie	8.05	eV	Cheméo Relay (1.0)
logp	4.223		Crippen Method
mcvol	276.650	ml/mol	McGowan Method
rinpol	2434.00		NIST Webbook
rinpol	2434.00		NIST Webbook
tb	666.95	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.45	J/mol×K	826.95	Joback Method
cpg	854.35	J/mol×K	862.81	Joback Method
cpg	870.02	J/mol×K	898.66	Joback Method
cpg	884.52	J/mol×K	934.52	Joback Method
cpg	897.91	J/mol×K	970.38	Joback Method
cpg	910.27	J/mol×K	1006.23	Joback Method
cpg	921.66	J/mol×K	1042.09	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C90540&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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