Diethylaminoethyl diphenylpropionate

Inchi: InChI=1S/C21H27NO2/c1-3-22(4-2)15-16-24-21(23)17-20(18-11-7-5-8-12-18)19-13-9-6-
InchiKey: ASQMSRQTKSSVSW-UHFFFAOYSA-N
Formula: C21H27NO2
SMILES: CCN(CC)CCOC(=O)CC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 325.44

Physical Properties

Property code	Value	Unit	Source
gf	225.18	kJ/mol	Joback Method
hf	-186.26	kJ/mol	Joback Method
hfus	40.51	kJ/mol	Joback Method
hvap	77.70	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.094		Crippen Method
mcvol	276.650	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
rinpol	2292.00		NIST Webbook
rinpol	2292.00		NIST Webbook
tb	821.53	K	Joback Method
tc	1038.79	K	Joback Method
tf	468.90	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.66	J/mol×K	821.53	Joback Method
cpg	855.88	J/mol×K	857.74	Joback Method
cpg	871.81	J/mol×K	893.95	Joback Method
cpg	886.53	J/mol×K	930.16	Joback Method
cpg	900.11	J/mol×K	966.37	Joback Method
cpg	912.63	J/mol×K	1002.58	Joback Method
cpg	924.17	J/mol×K	1038.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R17846&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume