

Succinic acid, phenyl N,N-diethyl-2-aminoethyl ester

Inchi: InChI=1S/C16H23NO4/c1-3-17(4-2)12-13-20-15(18)10-11-16(19)21-14-8-6-5-7-9-14/h5-9
InchiKey: UQFIQSKSOUCKAU-UHFFFAOYSA-N
Formula: C16H23NO4
SMILES: CCN(CC)CCOC(=O)CCC(=O)Oc1ccccc1
Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
gf	-160.81	kJ/mol	Joback Method
hf	-559.11	kJ/mol	Joback Method
hfus	39.83	kJ/mol	Joback Method
hvap	73.84	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.257		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
tb	757.18	K	Joback Method
tc	956.65	K	Joback Method
tf	473.29	K	Joback Method
vc	0.889	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.82	J/mol×K	757.18	Joback Method
cpg	705.14	J/mol×K	790.42	Joback Method
cpg	719.44	J/mol×K	823.67	Joback Method
cpg	732.75	J/mol×K	856.91	Joback Method
cpg	745.09	J/mol×K	890.16	Joback Method
cpg	756.49	J/mol×K	923.40	Joback Method
cpg	766.98	J/mol×K	956.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357998&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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