Succinic acid, 3,5-dinitro-4-methylbenzyl pentyl ester

Inchi: InChI=1S/C17H22N2O8/c1-3-4-5-8-26-16(20)6-7-17(21)27-11-13-9-14(18(22)23)12(2)15

InchiKey: YIQXSGUOBDRXPU-UHFFFAOYSA-N

Formula: C17H22N2O8

SMILES: CCCCCOC(=O)CCC(=O)OCc1cc([N+](=O)[O-])c(C)c([N+](=O)[O-])c1

Mol. weight [g/mol]: 382.37

Physical Properties

Property code	Value	Unit	Source
gf	-220.96	kJ/mol	Joback Method
hf	-703.21	kJ/mol	Joback Method
hfus	60.96	kJ/mol	Joback Method
hvap	109.19	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	3.368		Crippen Method
mcvol	276.350	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	2761.00		NIST Webbook
rinpol	2761.00		NIST Webbook
tb	1086.24	K	Joback Method
tc	1334.18	K	Joback Method
tf	776.87	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.13	J/mol×K	1086.24	Joback Method
cpg	904.75	J/mol×K	1127.56	Joback Method
cpg	910.84	J/mol×K	1168.89	Joback Method
cpg	915.42	J/mol×K	1210.21	Joback Method
cpg	918.53	J/mol×K	1251.53	Joback Method
cpg	920.19	J/mol×K	1292.85	Joback Method
cpg	920.41	J/mol×K	1334.18	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U382237&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/116-526-9/Succinic-acid-3-5-dinitro-4-methylbenzyl-pentyl-ester.pdf
Generated by Cheméo on 2024-05-03 06:20:43.279235169 +0000 UTC m=+17006492.199812480.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.