

Sebacic acid, 3-methyl-2-nitrobenzyl pentyl ester

Inchi:	InChI=1S/C23H35NO6/c1-3-4-11-17-29-21(25)15-9-7-5-6-8-10-16-22(26)30-18-20-14-12
InchiKey:	OVWFNPJROBKTBE-UHFFFAOYSA-N
Formula:	C23H35NO6
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OCc1cccc(C)c1[N+](=O)[O-]
Mol. weight [g/mol]:	421.53

Physical Properties

Property code	Value	Unit	Source
gf	-196.36	kJ/mol	Joback Method
hf	-804.82	kJ/mol	Joback Method
hfus	65.52	kJ/mol	Joback Method
hvap	105.30	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	5.801		Crippen Method
mcvol	343.470	ml/mol	McGowan Method
pc	1095.72	kPa	Joback Method
rinpola	3048.00		NIST Webbook
rinpola	3048.00		NIST Webbook
tb	1066.70	K	Joback Method
tc	1306.18	K	Joback Method
tf	688.36	K	Joback Method
vc	1.345	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1167.63	J/molxK	1066.70	Joback Method
cpg	1180.37	J/molxK	1106.61	Joback Method
cpg	1191.47	J/molxK	1146.53	Joback Method
cpg	1201.00	J/molxK	1186.44	Joback Method
cpg	1209.00	J/molxK	1226.35	Joback Method
cpg	1215.52	J/molxK	1266.27	Joback Method
cpg	1220.61	J/molxK	1306.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380733&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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