

Sebacic acid, butyl 4-nitrophenyl ester

Inchi:	InChI=1S/C20H29NO6/c1-2-3-16-26-19(22)10-8-6-4-5-7-9-11-20(23)27-18-14-12-17(13-
InchiKey:	BJYDFLDWAMTEEN-UHFFFAOYSA-N
Formula:	C20H29NO6
SMILES:	CCCCOC(=O)CCCCCCCC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	379.45

Physical Properties

Property code	Value	Unit	Source
gf	-211.99	kJ/mol	Joback Method
hf	-731.43	kJ/mol	Joback Method
hfus	58.14	kJ/mol	Joback Method
hvap	97.95	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	4.964		Crippen Method
mvol	301.200	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
rinpol	3040.00		NIST Webbook
rinpol	3040.00		NIST Webbook
tb	993.08	K	Joback Method
tc	1218.94	K	Joback Method
tf	642.03	K	Joback Method
vc	1.177	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.43	J/mol×K	993.08	Joback Method
cpg	1001.03	J/mol×K	1030.72	Joback Method
cpg	1012.27	J/mol×K	1068.37	Joback Method
cpg	1022.20	J/mol×K	1106.01	Joback Method
cpg	1030.85	J/mol×K	1143.65	Joback Method
cpg	1038.27	J/mol×K	1181.30	Joback Method
cpg	1044.48	J/mol×K	1218.94	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=U354786&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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