Sebacic acid, butyl 3-methyl-4-nitrobenzyl ester

Inchi: InChI=1S/C22H33NO6/c1-3-4-15-28-21(24)11-9-7-5-6-8-10-12-22(25)29-17-19-13-14-20

InchiKey: SXMNXPXBUSCTHR-UHFFFAOYSA-N

Formula: C22H33NO6

SMILES: CCCCOC(=O)CCCCCCCCC(=O)OCc1ccc([N+](=O)[O-])c(C)c1

Mol. weight [g/mol]: 407.50

Physical Properties

Property code	Value	Unit	Source
gf	-204.78	kJ/mol	Joback Method
hf	-784.18	kJ/mol	Joback Method
hfus	62.93	kJ/mol	Joback Method
hvap	103.07	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	5.411		Crippen Method
mcvol	329.380	ml/mol	McGowan Method
pc	1168.82	kPa	Joback Method
rinpol	3069.00		NIST Webbook
rinpol	3069.00		NIST Webbook
tb	1043.82	K	Joback Method
tc	1278.00	K	Joback Method
tf	677.09	K	Joback Method
vc	1.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.06	J/mol×K	1043.82	Joback Method
cpg	1119.70	J/mol×K	1082.85	Joback Method
cpg	1130.80	J/mol×K	1121.88	Joback Method
cpg	1140.40	J/mol×K	1160.91	Joback Method
cpg	1148.56	J/mol×K	1199.94	Joback Method
cpg	1155.30	J/mol×K	1238.97	Joback Method
cpg	1160.68	J/mol×K	1278.00	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=U380653&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