Terephthalic acid, butyl 4-nitro-3-methylbenzyl ester

Inchi: InChI=1S/C20H21NO6/c1-3-4-11-26-19(22)16-6-8-17(9-7-16)20(23)27-13-15-5-10-18(21

InchiKey: IZXQJWFMPNMJKA-UHFFFAOYSA-N

Formula: C20H21NO6

SMILES: CCCCOC(=O)c1ccc(C(=O)OCc2ccc([N+](=O)[O-])c(C)c2)cc1

Mol. weight [g/mol]: 371.38

Physical Properties

Property code	Value	Unit	Source
gf	-118.84	kJ/mol	Joback Method
hf	-517.84	kJ/mol	Joback Method
hfus	51.41	kJ/mol	Joback Method
hvap	101.56	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	4.217		Crippen Method
mcvol	277.440	ml/mol	McGowan Method
pc	1711.78	kPa	Joback Method
rinpol	3193.00		NIST Webbook
rinpol	3193.00		NIST Webbook
tb	1029.72	K	Joback Method
tc	1275.20	K	Joback Method
tf	693.49	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.20	J/mol×K	1029.72	Joback Method
cpg	883.85	J/mol×K	1070.63	Joback Method
cpg	892.03	J/mol×K	1111.55	Joback Method
cpg	898.79	J/mol×K	1152.46	Joback Method
cpg	904.15	J/mol×K	1193.38	Joback Method
cpg	908.17	J/mol×K	1234.29	Joback Method
cpg	910.87	J/mol×K	1275.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U416101&Units=SI

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