Phthalic acid, decyl 2-(2-nitrophenyl)ethyl ester

Inchi: InChI=1S/C26H33NO6/c1-2-3-4-5-6-7-8-13-19-32-25(28)22-15-10-11-16-23(22)26(29)33
InchiKey: MTXDHBGRHDPNLO-UHFFFAOYSA-N
Formula: C26H33NO6
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 455.54

Physical Properties

Property code	Value	Unit	Source
gf	-58.69	kJ/mol	Joback Method
hf	-630.21	kJ/mol	Joback Method
hfus	67.34	kJ/mol	Joback Method
hvap	114.25	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	6.292		Crippen Method
mcvol	361.980	ml/mol	McGowan Method
pc	1127.59	kPa	Joback Method
rinpol	3447.00		NIST Webbook
tb	1162.02	K	Joback Method
tc	1423.06	K	Joback Method
tf	748.59	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1231.72	J/mol×K	1162.02	Joback Method
cpg	1241.52	J/mol×K	1205.53	Joback Method
cpg	1249.63	J/mol×K	1249.03	Joback Method
cpg	1256.15	J/mol×K	1292.54	Joback Method
cpg	1261.17	J/mol×K	1336.05	Joback Method
cpg	1264.79	J/mol×K	1379.56	Joback Method
cpg	1267.10	J/mol×K	1423.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378000&Units=SI
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

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