Phenolphthalein, dibutyrate

Other names: (3-oxo-1(3H)-isobenzofurylidene)di-p-phenylene dibutyrate
Inchi: InChI=1S/C28H26O6/c1-3-9-25(29)32-21-13-7-11-19(17-21)28(24-16-6-5-15-23(24)27(3
InchiKey: LWUNSJOOQGPWSQ-UHFFFAOYSA-N
Formula: C28H26O6
SMILES: CCCC(=O)Oc1cccc(C2(c3cccc(OC(=O)CCC)c3)OC(=O)c3ccccc32)c1
Mol. weight [g/mol]: 458.50
CAS: 62625-15-4

Physical Properties

Property code	Value	Unit	Source
gf	-128.07	kJ/mol	Joback Method
hf	-617.33	kJ/mol	Joback Method
hfus	54.13	kJ/mol	Joback Method
hvap	112.57	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	5.560		Crippen Method
mcvol	345.560	ml/mol	McGowan Method
pc	1408.01	kPa	Joback Method
tb	1189.35	K	Joback Method
tc	1459.33	K	Joback Method
tf	803.09	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1209.85	J/mol×K	1189.35	Joback Method
cpg	1231.09	J/mol×K	1234.35	Joback Method
cpg	1252.81	J/mol×K	1279.34	Joback Method
cpg	1275.27	J/mol×K	1324.34	Joback Method
cpg	1298.73	J/mol×K	1369.33	Joback Method
cpg	1323.45	J/mol×K	1414.33	Joback Method
cpg	1349.68	J/mol×K	1459.33	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=C62625154&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume