Phthalic acid, 2-(2-bromophenyl)ethyl nonyl ester

Inchi: InChI=1S/C25H31BrO4/c1-2-3-4-5-6-7-12-18-29-24(27)21-14-9-10-15-22(21)25(28)30-19

InchiKey: VLYHUWWKLUGDEQ-UHFFFAOYSA-N

Formula: C25H31BrO4

SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1ccccc1Br

Mol. weight [g/mol]: 475.42

Physical Properties

Property code	Value	Unit	Source
gf	-88.34	kJ/mol	Joback Method
hf	-572.48	kJ/mol	Joback Method
hfus	58.67	kJ/mol	Joback Method
hvap	101.87	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	6.756		Crippen Method
mcvol	347.970	ml/mol	McGowan Method
pc	1253.03	kPa	Joback Method
rinpol	3167.00		NIST Webbook
rinpol	3167.00		NIST Webbook
tb	1053.46	K	Joback Method
tc	1291.53	K	Joback Method
tf	653.51	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1109.36	J/mol×K	1053.46	Joback Method
cpg	1121.95	J/mol×K	1093.14	Joback Method
cpg	1133.15	J/mol×K	1132.82	Joback Method
cpg	1143.03	J/mol×K	1172.49	Joback Method
cpg	1151.67	J/mol×K	1212.17	Joback Method
cpg	1159.15	J/mol×K	1251.85	Joback Method
cpg	1165.52	J/mol×K	1291.53	Joback Method
dvisc	0.0001770	Pa×s	653.51	Joback Method

dvisc	0.0001055	Pa×s	720.17	Joback Method
dvisc	0.0000687	Pa×s	786.83	Joback Method
dvisc	0.0000478	Pa×s	853.49	Joback Method
dvisc	0.0000351	Pa×s	920.14	Joback Method
dvisc	0.0000268	Pa×s	986.80	Joback Method
dvisc	0.0000212	Pa×s	1053.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377764&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
dvisc:	Dynamic viscosity
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