

Phthalic acid, 2-(4-bromophenyl)ethyl nonyl ester

Inchi:	InChI=1S/C25H31BrO4/c1-2-3-4-5-6-7-10-18-29-24(27)22-11-8-9-12-23(22)25(28)30-19
InchiKey:	HYZKODPHRMXPCV-UHFFFAOYSA-N
Formula:	C25H31BrO4
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1ccc(Br)cc1
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
mvol	347.970	ml/mol	McGowan Method
pc	1253.03	kPa	Joback Method
rinpol	3307.00		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/molxK	1053.46	Joback Method
cpg	1159.15	J/molxK	1251.85	Joback Method
cpg	1151.67	J/molxK	1212.17	Joback Method
cpg	1143.03	J/molxK	1172.49	Joback Method
cpg	1133.15	J/molxK	1132.82	Joback Method
cpg	1121.95	J/molxK	1093.14	Joback Method
cpg	1165.52	J/molxK	1291.53	Joback Method
dvisc	0.0000212	Paxs	1053.46	Joback Method
dvisc	0.0000268	Paxs	986.80	Joback Method

dvisc	0.0000351	Paxs	920.14	Joback Method
dvisc	0.0000478	Paxs	853.49	Joback Method
dvisc	0.0000687	Paxs	786.83	Joback Method
dvisc	0.0001055	Paxs	720.17	Joback Method
dvisc	0.0001770	Paxs	653.51	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U378042&Units=SI

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

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