

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

Inchi:	InChI=1S/C24H29BrO4/c1-2-3-4-5-6-9-17-28-23(26)21-10-7-8-11-22(21)24(27)29-18-16
InchiKey:	JRPXVNHTLABNFJ-UHFFFAOYSA-N
Formula:	C24H29BrO4
SMILES:	CCCCCCCCOC(=O)c1cccc1C(=O)OCCc1ccc(Br)cc1
Mol. weight [g/mol]:	461.39

Physical Properties

Property code	Value	Unit	Source
gf	-96.76	kJ/mol	Joback Method
hf	-551.84	kJ/mol	Joback Method
hfus	56.08	kJ/mol	Joback Method
hvap	99.64	kJ/mol	Joback Method
log10ws	-8.08		Crippen Method
logp	6.366		Crippen Method
mvol	333.880	ml/mol	McGowan Method
pc	1342.74	kPa	Joback Method
rinpol	3204.00		NIST Webbook
rinpol	3204.00		NIST Webbook
tb	1030.58	K	Joback Method
tc	1266.01	K	Joback Method
tf	642.24	K	Joback Method
vc	1.274	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.20	J/molxK	1030.58	Joback Method
cpg	1061.69	J/molxK	1069.82	Joback Method
cpg	1072.83	J/molxK	1109.06	Joback Method
cpg	1082.69	J/molxK	1148.29	Joback Method
cpg	1091.33	J/molxK	1187.53	Joback Method
cpg	1098.82	J/molxK	1226.77	Joback Method
cpg	1105.23	J/molxK	1266.01	Joback Method
dvisc	0.0001996	Paxs	642.24	Joback Method

dvisc	0.0001203	Paxs	706.96	Joback Method
dvisc	0.0000789	Paxs	771.69	Joback Method
dvisc	0.0000552	Paxs	836.41	Joback Method
dvisc	0.0000407	Paxs	901.13	Joback Method
dvisc	0.0000312	Paxs	965.86	Joback Method
dvisc	0.0000248	Paxs	1030.58	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=U378041&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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