

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

Inchi:	InChI=1S/C29H39BrO4/c1-2-3-4-5-6-7-8-9-10-11-14-22-33-28(31)26-15-12-13-16-27(26)
InchiKey:	YERGUNUHRSBGPM-UHFFFAOYSA-N
Formula:	C29H39BrO4
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCCc1ccc(Br)cc1
Mol. weight [g/mol]:	531.52

Physical Properties

Property code	Value	Unit	Source
gf	-54.66	kJ/mol	Joback Method
hf	-655.04	kJ/mol	Joback Method
hfus	69.03	kJ/mol	Joback Method
hvap	110.77	kJ/mol	Joback Method
log10ws	-10.18		Crippen Method
logp	8.316		Crippen Method
mcvol	404.330	ml/mol	McGowan Method
pc	971.09	kPa	Joback Method
rinsol	3705.00		NIST Webbook
rinsol	3705.00		NIST Webbook
tb	1144.98	K	Joback Method
tc	1404.80	K	Joback Method
tf	698.59	K	Joback Method
vc	1.554	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1353.95	J/molxK	1144.98	Joback Method
cpg	1367.14	J/molxK	1188.28	Joback Method
cpg	1378.70	J/molxK	1231.59	Joback Method
cpg	1388.76	J/molxK	1274.89	Joback Method
cpg	1397.43	J/molxK	1318.19	Joback Method
cpg	1404.82	J/molxK	1361.49	Joback Method
cpg	1411.07	J/molxK	1404.80	Joback Method
dvisc	0.0001067	Paxs	698.59	Joback Method

dvisc	0.0000613	Paxs	772.99	Joback Method
dvisc	0.0000388	Paxs	847.39	Joback Method
dvisc	0.0000264	Paxs	921.79	Joback Method
dvisc	0.0000191	Paxs	996.18	Joback Method
dvisc	0.0000144	Paxs	1070.58	Joback Method
dvisc	0.0000113	Paxs	1144.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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