

Diethylmalonic acid, 4-bromophenyl tetradecyl ester

Inchi:	InChI=1S/C27H43BrO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-22-31-25(29)27(5-2,6-3)26
InchiKey:	VQZFIJZTFGOPCJ-UHFFFAOYSA-N
Formula:	C27H43BrO4
SMILES:	CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	511.53

Physical Properties

Property code	Value	Unit	Source
gf	-171.44	kJ/mol	Joback Method
hf	-847.57	kJ/mol	Joback Method
hfus	62.78	kJ/mol	Joback Method
hvap	102.08	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	8.405		Crippen Method
mcvol	399.910	ml/mol	McGowan Method
pc	910.53	kPa	Joback Method
rinpol	3193.00		NIST Webbook
rinpol	3193.00		NIST Webbook
tb	1064.33	K	Joback Method
tc	1304.92	K	Joback Method
tf	639.53	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.92	J/molxK	1064.33	Joback Method
cpg	1362.39	J/molxK	1104.43	Joback Method
cpg	1377.46	J/molxK	1144.53	Joback Method
cpg	1391.24	J/molxK	1184.62	Joback Method
cpg	1403.85	J/molxK	1224.72	Joback Method
cpg	1415.39	J/molxK	1264.82	Joback Method
cpg	1425.98	J/molxK	1304.92	Joback Method
dvisc	0.0001381	Paxs	639.53	Joback Method

dvisc	0.0000729	Paxs	710.33	Joback Method
dvisc	0.0000432	Paxs	781.13	Joback Method
dvisc	0.0000280	Paxs	851.93	Joback Method
dvisc	0.0000193	Paxs	922.73	Joback Method
dvisc	0.0000141	Paxs	993.53	Joback Method
dvisc	0.0000107	Paxs	1064.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369831&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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