

Succinic acid, 3-bromophenethyl pentadecyl ester

Inchi:	InChI=1S/C27H43BrO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-21-31-26(29)18-19-27(30)32
InchiKey:	KLPMVWCTHWCHAN-UHFFFAOYSA-N
Formula:	C27H43BrO4
SMILES:	CCCCCCCCCCCCCOC(=O)CCC(=O)OCCc1cccc(Br)c1
Mol. weight [g/mol]:	511.53

Physical Properties

Property code	Value	Unit	Source
gf	-174.28	kJ/mol	Joback Method
hf	-838.82	kJ/mol	Joback Method
hfus	70.20	kJ/mol	Joback Method
hvap	103.38	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	7.949		Crippen Method
mcvol	399.910	ml/mol	McGowan Method
pc	900.18	kPa	Joback Method
rinpol	3432.00		NIST Webbook
rinpol	3432.00		NIST Webbook
tb	1067.56	K	Joback Method
tc	1312.05	K	Joback Method
tf	637.11	K	Joback Method
vc	1.550	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.75	J/molxK	1067.56	Joback Method
cpg	1362.06	J/molxK	1108.31	Joback Method
cpg	1376.71	J/molxK	1149.06	Joback Method
cpg	1389.79	J/molxK	1189.80	Joback Method
cpg	1401.38	J/molxK	1230.55	Joback Method
cpg	1411.59	J/molxK	1271.30	Joback Method
cpg	1420.49	J/molxK	1312.05	Joback Method
dvisc	0.0001655	Paxs	637.11	Joback Method

dvisc	0.0000897	Paxs	708.85	Joback Method
dvisc	0.0000544	Paxs	780.59	Joback Method
dvisc	0.0000359	Paxs	852.34	Joback Method
dvisc	0.0000253	Paxs	924.08	Joback Method
dvisc	0.0000187	Paxs	995.82	Joback Method
dvisc	0.0000144	Paxs	1067.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381292&Units=SI
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

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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