

Succinic acid, 3-bromobenzyl tridecyl ester

Inchi: InChI=1S/C24H37BrO4/c1-2-3-4-5-6-7-8-9-10-11-12-18-28-23(26)16-17-24(27)29-20-21
InchiKey: AGTTYJMJQSKOAI-UHFFFAOYSA-N
Formula: C24H37BrO4
SMILES: CCCCCCCCCCCCCOC(=O)CCC(=O)OCc1cccc(Br)c1
Mol. weight [g/mol]: 469.45

Physical Properties

Property code	Value	Unit	Source
gf	-199.54	kJ/mol	Joback Method
hf	-776.90	kJ/mol	Joback Method
hfus	62.43	kJ/mol	Joback Method
hvap	96.70	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	7.127		Crippen Method
mcvol	357.640	ml/mol	McGowan Method
pc	1078.51	kPa	Joback Method
rinpol	3135.00		NIST Webbook
rinpol	3135.00		NIST Webbook
tb	998.92	K	Joback Method
tc	1222.96	K	Joback Method
tf	603.30	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1159.59	J/molxK	998.92	Joback Method
cpg	1223.25	J/molxK	1185.62	Joback Method
cpg	1213.05	J/molxK	1148.28	Joback Method
cpg	1201.64	J/molxK	1110.94	Joback Method
cpg	1188.96	J/molxK	1073.60	Joback Method
cpg	1174.96	J/molxK	1036.26	Joback Method
cpg	1232.30	J/molxK	1222.96	Joback Method
dvisc	0.0000232	Paxs	998.92	Joback Method

dvisc	0.0000299	Paxs	932.98	Joback Method
dvisc	0.0000400	Paxs	867.05	Joback Method
dvisc	0.0000562	Paxs	801.11	Joback Method
dvisc	0.0000838	Paxs	735.17	Joback Method
dvisc	0.0001353	Paxs	669.24	Joback Method
dvisc	0.0002425	Paxs	603.30	Joback Method

Sources

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=U382424&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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