

Succinic acid, di(3-bromophenethyl) ester

Inchi: InChI=1S/C20H20Br2O4/c21-17-5-1-3-15(13-17)9-11-25-19(23)7-8-20(24)26-12-10-16-4
InchiKey: HVOKIDPRZHDPMV-UHFFFAOYSA-N
Formula: C20H20Br2O4
SMILES: O=C(CCC(=O)OCCc1cccc(Br)c1)OCCc1cccc(Br)c1
Mol. weight [g/mol]: 484.18

Physical Properties

Property code	Value	Unit	Source
gf	-116.12	kJ/mol	Joback Method
hf	-442.95	kJ/mol	Joback Method
hfus	51.00	kJ/mol	Joback Method
hvap	97.17	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	4.863		Crippen Method
mvol	295.020	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	3170.00		NIST Webbook
rinpol	3170.00		NIST Webbook
tb	1005.22	K	Joback Method
tc	1249.21	K	Joback Method
tf	656.96	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.62	J/molxK	1005.22	Joback Method
cpg	883.91	J/molxK	1208.55	Joback Method
cpg	877.68	J/molxK	1167.88	Joback Method
cpg	870.50	J/molxK	1127.22	Joback Method
cpg	862.31	J/molxK	1086.55	Joback Method
cpg	853.04	J/molxK	1045.89	Joback Method
cpg	889.27	J/molxK	1249.21	Joback Method
dvisc	0.0000342	Paxs	1005.22	Joback Method

dvisc	0.0000422	Paxs	947.18	Joback Method
dvisc	0.0000536	Paxs	889.13	Joback Method
dvisc	0.0000704	Paxs	831.09	Joback Method
dvisc	0.0000963	Paxs	773.05	Joback Method
dvisc	0.0001385	Paxs	715.00	Joback Method
dvisc	0.0002125	Paxs	656.96	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=U381293&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
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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