

Succinic acid, 2-bromophenethyl butyl ester

Inchi: InChI=1S/C16H21BrO4/c1-2-3-11-20-15(18)8-9-16(19)21-12-10-13-6-4-5-7-14(13)17/h4-19
InchiKey: STSPDLAHXWFLMN-UHFFFAOYSA-N
Formula: C16H21BrO4
SMILES: CCCOC(=O)CCC(=O)OCCc1ccccc1Br
Mol. weight [g/mol]: 357.24

Physical Properties

Property code	Value	Unit	Source
gf	-266.90	kJ/mol	Joback Method
hf	-611.78	kJ/mol	Joback Method
hfus	41.71	kJ/mol	Joback Method
hvap	78.90	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.658		Crippen Method
mcvol	244.920	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	2320.00		NIST Webbook
rinpol	2320.00		NIST Webbook
tb	815.88	K	Joback Method
tc	1027.86	K	Joback Method
tf	513.14	K	Joback Method
vc	0.933	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.61	J/molxK	815.88	Joback Method
cpg	701.14	J/molxK	851.21	Joback Method
cpg	713.65	J/molxK	886.54	Joback Method
cpg	725.19	J/molxK	921.87	Joback Method
cpg	735.77	J/molxK	957.20	Joback Method
cpg	745.41	J/molxK	992.53	Joback Method
cpg	754.13	J/molxK	1027.86	Joback Method
dvisc	0.0005914	Paxs	513.14	Joback Method

dvisc	0.0003615	Paxs	563.60	Joback Method
dvisc	0.0002396	Paxs	614.05	Joback Method
dvisc	0.0001691	Paxs	664.51	Joback Method
dvisc	0.0001253	Paxs	714.97	Joback Method
dvisc	0.0000966	Paxs	765.42	Joback Method
dvisc	0.0000769	Paxs	815.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381449&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_cvol:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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