Succinic acid, 7-bromoheptyl pentyl ester

Inchi: InChI=1S/C16H29BrO4/c1-2-3-8-13-20-15(18)10-11-16(19)21-14-9-6-4-5-7-12-17/h2-14
InchiKey: RICSTKIZGNZGGP-UHFFFAOYSA-N
Formula: C16H29BrO4
SMILES: CCCCCOC(=O)CCC(=O)OCCCCCCCBr
Mol. weight [g/mol]: 365.30

Physical Properties

Property code	Value	Unit	Source
gf	-369.68	kJ/mol	Joback Method
hf	-836.84	kJ/mol	Joback Method
hfus	48.05	kJ/mol	Joback Method
hvap	75.96	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.389		Crippen Method
mcvol	268.680	ml/mol	McGowan Method
pc	1487.29	kPa	Joback Method
rinpol	2342.00		NIST Webbook
rinpol	2342.00		NIST Webbook
tb	784.22	K	Joback Method
tc	971.96	K	Joback Method
tf	474.20	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.43	J/mol×K	784.22	Joback Method
cpg	795.78	J/mol×K	815.51	Joback Method
cpg	810.24	J/mol×K	846.80	Joback Method
cpg	823.84	J/mol×K	878.09	Joback Method
cpg	836.60	J/mol×K	909.38	Joback Method
cpg	848.52	J/mol×K	940.67	Joback Method
cpg	859.62	J/mol×K	971.96	Joback Method
dvisc	0.0007993	Pa×s	474.20	Joback Method

dvisc	0.0004439	Pa×s	525.87	Joback Method
dvisc	0.0002739	Pa×s	577.54	Joback Method
dvisc	0.0001829	Pa×s	629.21	Joback Method
dvisc	0.0001299	Pa×s	680.88	Joback Method
dvisc	0.0000968	Pa×s	732.55	Joback Method
dvisc	0.0000750	Pa×s	784.22	Joback Method

Sources

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=U382406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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