Succinic acid, 7-bromoheptyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H33BrO4/c1-4-10-16(15(2)3)23-18(21)12-11-17(20)22-14-9-7-5-6-8-13-19/

InchiKey: ZGVHYXMWVYVHFB-UHFFFAOYSA-N

Formula: C18H33BrO4

SMILES: CCCC(OC(=O)CCC(=O)OCCCCCCCBr)C(C)C

Mol. weight [g/mol]: 393.36

Physical Properties

Property code	Value	Unit	Source
gf	-357.72	kJ/mol	Joback Method
hf	-888.68	kJ/mol	Joback Method
hfus	46.19	kJ/mol	Joback Method
hvap	79.63	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.023		Crippen Method
mcvol	296.860	ml/mol	McGowan Method
pc	1304.23	kPa	Joback Method
rinpol	2440.00		NIST Webbook
rinpol	2440.00		NIST Webbook
tb	829.10	K	Joback Method
tc	1022.40	K	Joback Method
tf	466.74	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.14	J/mol×K	829.10	Joback Method
cpg	969.58	J/mol×K	990.18	Joback Method
cpg	957.25	J/mol×K	957.96	Joback Method
cpg	943.97	J/mol×K	925.75	Joback Method
cpg	929.70	J/mol×K	893.53	Joback Method
cpg	914.43	J/mol×K	861.32	Joback Method
cpg	980.97	J/mol×K	1022.40	Joback Method
dvisc	0.0000469	Pa×s	829.10	Joback Method

dvisc	0.0000629	Pa×s	768.71	Joback Method
dvisc	0.0000888	Pa×s	708.31	Joback Method
dvisc	0.0001335	Pa×s	647.92	Joback Method
dvisc	0.0002184	Pa×s	587.53	Joback Method
dvisc	0.0004000	Pa×s	527.13	Joback Method
dvisc	0.0008566	Pa×s	466.74	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=U382407&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