Sebacic acid, butyl octyl ester

Inchi: InChI=1S/C22H42O4/c1-3-5-7-8-13-16-20-26-22(24)18-15-12-10-9-11-14-17-21(23)25-1
InchiKey: LPUVPRFNUDDWIA-UHFFFAOYSA-N
Formula: C22H42O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]: 370.57

Physical Properties

Property code	Value	Unit	Source
gf	-333.48	kJ/mol	Joback Method
hf	-987.01	kJ/mol	Joback Method
hfus	58.31	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.354		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	953.78	kPa	Joback Method
rinpol	2628.00		NIST Webbook
tb	855.34	K	Joback Method
tc	1047.20	K	Joback Method
tf	482.02	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.06	J/mol×K	855.34	Joback Method
cpg	1111.23	J/mol×K	887.32	Joback Method
cpg	1129.19	J/mol×K	919.29	Joback Method
cpg	1145.99	J/mol×K	951.27	Joback Method
cpg	1161.63	J/mol×K	983.25	Joback Method
cpg	1176.14	J/mol×K	1015.23	Joback Method
cpg	1189.55	J/mol×K	1047.20	Joback Method
dvisc	0.0006693	Pa×s	482.02	Joback Method
dvisc	0.0003195	Pa×s	544.24	Joback Method

dvisc	0.0001775	Pa×s	606.46	Joback Method
dvisc	0.0001100	Pa×s	668.68	Joback Method
dvisc	0.0000739	Pa×s	730.90	Joback Method
dvisc	0.0000529	Pa×s	793.12	Joback Method
dvisc	0.0000397	Pa×s	855.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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