Sebacic acid, isohexyl 2-methoxyethyl ester

Inchi: InChI=1S/C19H36O5/c1-17(2)11-10-14-23-18(20)12-8-6-4-5-7-9-13-19(21)24-16-15-22-3
InchiKey: UPFNIFNYOOEFOC-UHFFFAOYSA-N
Formula: C19H36O5
SMILES: COCCOC(=O)CCCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 344.49

Physical Properties

Property code	Value	Unit	Source
gf	-466.18	kJ/mol	Joback Method
hf	-1062.59	kJ/mol	Joback Method
hfus	48.20	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.276		Crippen Method
mcvol	299.320	ml/mol	McGowan Method
pc	1142.12	kPa	Joback Method
rinpol	2379.00		NIST Webbook
tb	808.68	K	Joback Method
tc	993.30	K	Joback Method
tf	455.44	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.75	J/mol×K	808.68	Joback Method
cpg	958.44	J/mol×K	839.45	Joback Method
cpg	975.07	J/mol×K	870.22	Joback Method
cpg	990.65	J/mol×K	900.99	Joback Method
cpg	1005.16	J/mol×K	931.76	Joback Method
cpg	1018.64	J/mol×K	962.53	Joback Method
cpg	1031.06	J/mol×K	993.30	Joback Method
dvisc	0.0007490	Pa×s	455.44	Joback Method
dvisc	0.0003527	Pa×s	514.31	Joback Method

dvisc	0.0001939	Pa×s	573.19	Joback Method
dvisc	0.0001192	Pa×s	632.06	Joback Method
dvisc	0.0000796	Pa×s	690.93	Joback Method
dvisc	0.0000566	Pa×s	749.81	Joback Method
dvisc	0.0000423	Pa×s	808.68	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355757&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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