Sebacic acid, 4-heptyl isobutyl ester

Inchi: InChI=1S/C21H40O4/c1-5-13-19(14-6-2)25-21(23)16-12-10-8-7-9-11-15-20(22)24-17-18
InchiKey: WWPHUQVOGNLDRG-UHFFFAOYSA-N
Formula: C21H40O4
SMILES: CCCC(CCC)OC(=O)CCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	-346.78	kJ/mol	Joback Method
hf	-976.93	kJ/mol	Joback Method
hfus	48.67	kJ/mol	Joback Method
hvap	79.88	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.818		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1023.34	kPa	Joback Method
rinpol	2319.00		NIST Webbook
tb	831.58	K	Joback Method
tc	1019.89	K	Joback Method
tf	440.75	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.20	J/mol×K	831.58	Joback Method
cpg	1113.87	J/mol×K	988.51	Joback Method
cpg	1099.54	J/mol×K	957.12	Joback Method
cpg	1084.13	J/mol×K	925.74	Joback Method
cpg	1067.62	J/mol×K	894.35	Joback Method
cpg	1049.98	J/mol×K	862.97	Joback Method
cpg	1127.14	J/mol×K	1019.89	Joback Method
dvisc	0.0000387	Pa×s	831.58	Joback Method
dvisc	0.0000532	Pa×s	766.44	Joback Method

dvisc	0.0000774	Pa×s	701.30	Joback Method
dvisc	0.0001217	Pa×s	636.16	Joback Method
dvisc	0.0002123	Pa×s	571.03	Joback Method
dvisc	0.0004270	Pa×s	505.89	Joback Method
dvisc	0.0010562	Pa×s	440.75	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=U355383&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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