Sebacic acid, hexyl pent-4-enyl ester

Inchi: InChI=1S/C21H38O4/c1-3-5-7-15-19-25-21(23)17-13-11-9-8-10-12-16-20(22)24-18-14-6
InchiKey: XVIGGHIBKXBZAQ-UHFFFAOYSA-N
Formula: C21H38O4
SMILES: C=CCCCOC(=O)CCCCCCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-254.06	kJ/mol	Joback Method
hf	-840.94	kJ/mol	Joback Method
hfus	54.44	kJ/mol	Joback Method
hvap	79.98	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.740		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1040.58	kPa	Joback Method
rinpol	2488.00		NIST Webbook
rinpol	2488.00		NIST Webbook
tb	829.14	K	Joback Method
tc	1016.39	K	Joback Method
tf	468.99	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.79	J/mol×K	829.14	Joback Method
cpg	1082.97	J/mol×K	985.18	Joback Method
cpg	1068.99	J/mol×K	953.97	Joback Method
cpg	1054.00	J/mol×K	922.77	Joback Method
cpg	1037.99	J/mol×K	891.56	Joback Method
cpg	1020.92	J/mol×K	860.35	Joback Method
cpg	1095.98	J/mol×K	1016.39	Joback Method
dvisc	0.0000493	Pa×s	829.14	Joback Method

dvisc	0.0000651	Pa×s	769.12	Joback Method
dvisc	0.0000902	Pa×s	709.09	Joback Method
dvisc	0.0001326	Pa×s	649.07	Joback Method
dvisc	0.0002110	Pa×s	589.04	Joback Method
dvisc	0.0003732	Pa×s	529.01	Joback Method
dvisc	0.0007636	Pa×s	468.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355413&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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