

Sebacic acid, but-2-enyl octyl ester

Inchi:	InChI=1S/C22H40O4/c1-3-5-7-8-13-16-20-26-22(24)18-15-12-10-9-11-14-17-21(23)25-1
InchiKey:	SBCYPQAMQMRAEP-GQCTYLIASA-N
Formula:	C22H40O4
SMILES:	CC=CCOC(=O)CCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]:	368.55

Physical Properties

Property code	Value	Unit	Source
gf	-253.26	kJ/mol	Joback Method
hf	-869.79	kJ/mol	Joback Method
hfus	58.51	kJ/mol	Joback Method
hvap	82.84	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.130		Crippen Method
mvol	331.420	ml/mol	McGowan Method
pc	985.16	kPa	Joback Method
rinpol	2587.00		NIST Webbook
rinpol	2587.00		NIST Webbook
tb	859.50	K	Joback Method
tc	1052.62	K	Joback Method
tf	476.94	K	Joback Method
vc	1.296	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.82	J/molxK	859.50	Joback Method
cpg	1084.38	J/molxK	891.69	Joback Method
cpg	1101.82	J/molxK	923.87	Joback Method
cpg	1118.16	J/molxK	956.06	Joback Method
cpg	1133.46	J/molxK	988.25	Joback Method
cpg	1147.73	J/molxK	1020.43	Joback Method
cpg	1161.02	J/molxK	1052.62	Joback Method
dvisc	0.0006226	Paxs	476.94	Joback Method

dvisc	0.0002897	Paxs	540.70	Joback Method
dvisc	0.0001584	Paxs	604.46	Joback Method
dvisc	0.0000972	Paxs	668.22	Joback Method
dvisc	0.0000649	Paxs	731.98	Joback Method
dvisc	0.0000463	Paxs	795.74	Joback Method
dvisc	0.0000347	Paxs	859.50	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U355908&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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