Sebacic acid, 3-methylbut-3-enyl pentyl ester

Inchi: InChI=1S/C20H36O4/c1-4-5-12-16-23-19(21)13-10-8-6-7-9-11-14-20(22)24-17-15-18(2)3
InchiKey: NISFNGJNUDWKDD-UHFFFAOYSA-N
Formula: C20H36O4
SMILES: C=C(C)CCOC(=O)CCCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-271.03	kJ/mol	Joback Method
hf	-830.09	kJ/mol	Joback Method
hfus	50.54	kJ/mol	Joback Method
hvap	77.84	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.350		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	2369.00		NIST Webbook
tb	806.14	K	Joback Method
tc	990.90	K	Joback Method
tf	443.76	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.86	J/mol×K	806.14	Joback Method
cpg	959.64	J/mol×K	836.93	Joback Method
cpg	976.40	J/mol×K	867.73	Joback Method
cpg	992.17	J/mol×K	898.52	Joback Method
cpg	1006.97	J/mol×K	929.31	Joback Method
cpg	1020.83	J/mol×K	960.10	Joback Method
cpg	1033.76	J/mol×K	990.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355935&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
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