Sebacic acid, di(3-methylbut-3-enyl) ester

Inchi: InChI=1S/C20H34O4/c1-17(2)13-15-23-19(21)11-9-7-5-6-8-10-12-20(22)24-16-14-18(3)4
InchiKey: TUQYJYUXCPBEGU-UHFFFAOYSA-N
Formula: C20H34O4
SMILES: C=C(C)CCOC(=O)CCCCCCCCC(=O)OCCC(=C)C
Mol. weight [g/mol]: 338.48

Physical Properties

Property code	Value	Unit	Source
gf	-191.74	kJ/mol	Joback Method
hf	-714.45	kJ/mol	Joback Method
hfus	47.95	kJ/mol	Joback Method
hvap	77.25	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.126		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
tb	802.70	K	Joback Method
tc	988.99	K	Joback Method
tf	428.04	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.69	J/mol×K	802.70	Joback Method
cpg	932.01	J/mol×K	833.75	Joback Method
cpg	948.35	J/mol×K	864.80	Joback Method
cpg	963.73	J/mol×K	895.84	Joback Method
cpg	978.17	J/mol×K	926.89	Joback Method
cpg	991.70	J/mol×K	957.94	Joback Method
cpg	1004.35	J/mol×K	988.99	Joback Method

Sources

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=U355948&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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