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

Inchi: InChI=1S/C19H34O4/c1-16(2)13-14-22-18(20)11-9-7-5-6-8-10-12-19(21)23-15-17(3)4/h1

InchiKey: ARMDGGLDMQRCHJ-UHFFFAOYSA-N

Formula: C19H34O4

SMILES: C=C(C)CCOC(=O)CCCCCCCCC(=O)OCC(C)C

Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-281.89	kJ/mol	Joback Method
hf	-814.73	kJ/mol	Joback Method
hfus	44.43	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.816		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	2221.00		NIST Webbook
tb	782.82	K	Joback Method
tc	966.60	K	Joback Method
tf	417.49	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.64	J/mol×K	782.82	Joback Method
cpg	900.14	J/mol×K	813.45	Joback Method
cpg	916.67	J/mol×K	844.08	Joback Method
cpg	932.25	J/mol×K	874.71	Joback Method
cpg	946.88	J/mol×K	905.34	Joback Method
cpg	960.59	J/mol×K	935.97	Joback Method
cpg	973.40	J/mol×K	966.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355933&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