Sebacic acid, butyl 3-methylbut-2-enyl ester

Inchi: InChI=1S/C19H34O4/c1-4-5-15-22-18(20)12-10-8-6-7-9-11-13-19(21)23-16-14-17(2)3/h1
InchiKey: BACNIACDBAYFEW-UHFFFAOYSA-N
Formula: C19H34O4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-287.07	kJ/mol	Joback Method
hf	-817.66	kJ/mol	Joback Method
hfus	49.43	kJ/mol	Joback Method
hvap	76.24	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.960		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1194.82	kPa	Joback Method
rinpol	2300.00		NIST Webbook
tb	790.74	K	Joback Method
tc	975.58	K	Joback Method
tf	429.17	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.72	J/mol×K	790.74	Joback Method
cpg	901.08	J/mol×K	821.55	Joback Method
cpg	917.50	J/mol×K	852.35	Joback Method
cpg	932.99	J/mol×K	883.16	Joback Method
cpg	947.57	J/mol×K	913.97	Joback Method
cpg	961.28	J/mol×K	944.77	Joback Method
cpg	974.14	J/mol×K	975.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355877&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
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