Sebacic acid, di(but-3-yn-2-yl) ester

Inchi: InChI=1S/C18H26O4/c1-5-15(3)21-17(19)13-11-9-7-8-10-12-14-18(20)22-16(4)6-2/h1-2,
InchiKey: BZAIQLWYPRLMJI-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: C#CC(C)OC(=O)CCCCCCCCC(=O)OC(C)C#C
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	74.10	kJ/mol	Joback Method
hf	-331.21	kJ/mol	Joback Method
hfus	46.85	kJ/mol	Joback Method
hvap	72.91	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.237		Crippen Method
mcvol	262.160	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	2031.00		NIST Webbook
tb	743.18	K	Joback Method
tc	936.10	K	Joback Method
tf	500.88	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.93	J/mol×K	743.18	Joback Method
cpg	761.79	J/mol×K	775.33	Joback Method
cpg	776.75	J/mol×K	807.49	Joback Method
cpg	790.83	J/mol×K	839.64	Joback Method
cpg	804.06	J/mol×K	871.79	Joback Method
cpg	816.45	J/mol×K	903.94	Joback Method
cpg	828.03	J/mol×K	936.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355853&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