Sebacic acid, but-3-yn-2-yl heptyl ester

Inchi: InChI=1S/C21H36O4/c1-4-6-7-12-15-18-24-20(22)16-13-10-8-9-11-14-17-21(23)25-19(3
InchiKey: ZWUGXFSXWITRHH-UHFFFAOYSA-N
Formula: C21H36O4
SMILES: C#CC(C)OC(=O)CCCCCCCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-121.27	kJ/mol	Joback Method
hf	-679.75	kJ/mol	Joback Method
hfus	55.17	kJ/mol	Joback Method
hvap	80.12	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	5.186		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1121.55	kPa	Joback Method
rinpol	2391.00		NIST Webbook
rinpol	2391.00		NIST Webbook
tb	822.14	K	Joback Method
tc	1010.84	K	Joback Method
tf	502.72	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.11	J/mol×K	822.14	Joback Method
cpg	991.77	J/mol×K	853.59	Joback Method
cpg	1008.39	J/mol×K	885.04	Joback Method
cpg	1023.99	J/mol×K	916.49	Joback Method
cpg	1038.59	J/mol×K	947.94	Joback Method
cpg	1052.22	J/mol×K	979.39	Joback Method
cpg	1064.90	J/mol×K	1010.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355849&Units=SI

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