Diethyl, dipropargyl malonate

Inchi: InChI=1S/C13H16O4/c1-5-9-13(10-6-2,11(14)16-7-3)12(15)17-8-4/h1-2H,7-10H2,3-4H3
InchiKey: MYZCCWFBKBDURM-UHFFFAOYSA-N
Formula: C13H16O4
SMILES: C#CCC(CC#C)(C(=O)OCC)C(=O)OCC
Mol. weight [g/mol]: 236.26
CAS: 2689-88-5

Physical Properties

Property code	Value	Unit	Source
gf	39.72	kJ/mol	Joback Method
hf	-226.20	kJ/mol	Joback Method
hfus	33.54	kJ/mol	Joback Method
hvap	61.26	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.146		Crippen Method
mcvol	191.710	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
tb	626.43	K	Joback Method
tc	832.14	K	Joback Method
tf	476.95	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.82	J/mol×K	626.43	Joback Method
cpg	496.29	J/mol×K	660.71	Joback Method
cpg	508.95	J/mol×K	695.00	Joback Method
cpg	520.84	J/mol×K	729.28	Joback Method
cpg	532.00	J/mol×K	763.57	Joback Method
cpg	542.44	J/mol×K	797.85	Joback Method
cpg	552.20	J/mol×K	832.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2689885&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume