Diethylmalonic acid, heptyl tetrahydrofurfuryl ester

Inchi: InChI=1S/C19H34O5/c1-4-7-8-9-10-13-23-17(20)19(5-2,6-3)18(21)24-15-16-12-11-14-22

InchiKey: PIHTYHCJVUHJIG-UHFFFAOYSA-N

Formula: C19H34O5

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OCC1CCCO1

Mol. weight [g/mol]: 342.47

Physical Properties

Property code	Value	Unit	Source
gf	-405.47	kJ/mol	Joback Method
hf	-1005.36	kJ/mol	Joback Method
hfus	45.04	kJ/mol	Joback Method
hvap	79.67	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.029		Crippen Method
mcvol	288.460	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpol	2151.00		NIST Webbook
rinpol	2151.00		NIST Webbook
tb	825.70	K	Joback Method
tc	1023.88	K	Joback Method
tf	488.10	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.60	J/mol×K	825.70	Joback Method
cpg	955.46	J/mol×K	858.73	Joback Method
cpg	972.12	J/mol×K	891.76	Joback Method
cpg	987.63	J/mol×K	924.79	Joback Method
cpg	1002.04	J/mol×K	957.82	Joback Method
cpg	1015.37	J/mol×K	990.85	Joback Method
cpg	1027.67	J/mol×K	1023.88	Joback Method
dvisc	0.0009216	Pa×s	488.10	Joback Method

dvisc	0.0004666	Pa×s	544.37	Joback Method
dvisc	0.0002684	Pa×s	600.63	Joback Method
dvisc	0.0001697	Pa×s	656.90	Joback Method
dvisc	0.0001153	Pa×s	713.17	Joback Method
dvisc	0.0000830	Pa×s	769.43	Joback Method
dvisc	0.0000624	Pa×s	825.70	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=U370642&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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