

Diethylmalonic acid, octyl tetrahydrofurfuryl ester

Inchi:	InChI=1S/C20H36O5/c1-4-7-8-9-10-11-14-24-18(21)20(5-2,6-3)19(22)25-16-17-13-12-15
InchiKey:	DYJPLVPIGIBPIZ-UHFFFAOYSA-N
Formula:	C20H36O5
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC1CCCO1
Mol. weight [g/mol]:	356.50

Physical Properties

Property code	Value	Unit	Source
gf	-397.05	kJ/mol	Joback Method
hf	-1026.00	kJ/mol	Joback Method
hfus	47.63	kJ/mol	Joback Method
hvap	81.90	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.419		Crippen Method
mvol	302.550	ml/mol	McGowan Method
pc	1225.98	kPa	Joback Method
rinpol	2265.00		NIST Webbook
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tb	848.58	K	Joback Method
tc	1047.72	K	Joback Method
tf	499.37	K	Joback Method
vc	1.155	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.90	J/molxK	848.58	Joback Method
cpg	1076.20	J/molxK	1014.53	Joback Method
cpg	1062.81	J/molxK	981.34	Joback Method
cpg	1048.33	J/molxK	948.15	Joback Method
cpg	1032.72	J/molxK	914.96	Joback Method
cpg	1015.93	J/molxK	881.77	Joback Method
cpg	1088.53	J/molxK	1047.72	Joback Method
dvisc	0.0000536	Paxs	848.58	Joback Method

dvisc	0.0000714	Paxs	790.38	Joback Method
dvisc	0.0000995	Paxs	732.18	Joback Method
dvisc	0.0001471	Paxs	673.97	Joback Method
dvisc	0.0002339	Paxs	615.77	Joback Method
dvisc	0.0004098	Paxs	557.57	Joback Method
dvisc	0.0008183	Paxs	499.37	Joback Method

Sources

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=U370643&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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

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