

Diethylmalonic acid, heptyl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C20H38O4/c1-7-10-11-12-13-14-23-18(21)20(8-2,9-3)19(22)24-17(6)15-16(4)5
InchiKey:	HSQVQSXDIXYARZ-UHFFFAOYSA-N
Formula:	C20H38O4
SMILES:	CCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)CC(C)C
Mol. weight [g/mol]:	342.51

Physical Properties

Property code	Value	Unit	Source
gf	-352.36	kJ/mol	Joback Method
hf	-965.04	kJ/mol	Joback Method
hfus	38.67	kJ/mol	Joback Method
hvap	76.35	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.284		Crippen Method
mvol	307.540	ml/mol	McGowan Method
pc	1103.01	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook
tb	805.47	K	Joback Method
tc	993.66	K	Joback Method
tf	431.90	K	Joback Method
vc	1.181	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.15	J/molxK	805.47	Joback Method
cpg	989.61	J/molxK	836.83	Joback Method
cpg	1006.98	J/molxK	868.20	Joback Method
cpg	1023.29	J/molxK	899.56	Joback Method
cpg	1038.57	J/molxK	930.93	Joback Method
cpg	1052.84	J/molxK	962.29	Joback Method
cpg	1066.15	J/molxK	993.66	Joback Method
dvisc	0.0011766	Paxs	431.90	Joback Method

dvisc	0.0004564	Paxs	494.16	Joback Method
dvisc	0.0002188	Paxs	556.42	Joback Method
dvisc	0.0001216	Paxs	618.68	Joback Method
dvisc	0.0000753	Paxs	680.95	Joback Method
dvisc	0.0000505	Paxs	743.21	Joback Method
dvisc	0.0000360	Paxs	805.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U370500&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

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