

Diethylmalonic acid, heptyl 2-methylpentyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-349.92	kJ/mol	Joback Method
hf	-959.76	kJ/mol	Joback Method
hfus	42.19	kJ/mol	Joback Method
hvap	76.74	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	5.286		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinsol	1963.00		NIST Webbook
tb	805.91	K	Joback Method
tc	992.86	K	Joback Method
tf	446.90	K	Joback Method
vc	1.187	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.67	J/molxK	805.91	Joback Method
cpg	1051.98	J/molxK	961.70	Joback Method
cpg	1037.73	J/molxK	930.54	Joback Method
cpg	1022.51	J/molxK	899.38	Joback Method
cpg	1006.28	J/molxK	868.23	Joback Method
cpg	989.01	J/molxK	837.07	Joback Method
cpg	1065.27	J/molxK	992.86	Joback Method
dvisc	0.0000392	Paxs	805.91	Joback Method
dvisc	0.0000540	Paxs	746.08	Joback Method

dvisc	0.0000785	Paxs	686.24	Joback Method
dvisc	0.0001227	Paxs	626.40	Joback Method
dvisc	0.0002108	Paxs	566.57	Joback Method
dvisc	0.0004114	Paxs	506.73	Joback Method
dvisc	0.0009605	Paxs	446.90	Joback Method

Sources

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=U369760&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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