

Ethane-1,2-diyl bis(3,5,5-trimethylhexanoate)

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

Physical Properties

Property code	Value	Unit	Source
gf	-349.52	kJ/mol	Joback Method
hf	-973.79	kJ/mol	Joback Method
hfus	31.26	kJ/mol	Joback Method
hvap	75.06	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.998		Crippen Method
mvol	307.540	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
rinpol	2028.00		NIST Webbook
rinpol	2028.00		NIST Webbook
tb	802.24	K	Joback Method
tc	994.46	K	Joback Method
tf	434.32	K	Joback Method
vc	1.169	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.22	J/molxK	802.24	Joback Method
cpg	990.84	J/molxK	834.28	Joback Method
cpg	1008.33	J/molxK	866.31	Joback Method
cpg	1024.74	J/molxK	898.35	Joback Method
cpg	1040.11	J/molxK	930.39	Joback Method
cpg	1054.51	J/molxK	962.43	Joback Method
cpg	1067.96	J/molxK	994.46	Joback Method
dvisc	0.0011509	Paxs	434.32	Joback Method

dvisc	0.0004263	Paxs	495.64	Joback Method
dvisc	0.0001965	Paxs	556.96	Joback Method
dvisc	0.0001056	Paxs	618.28	Joback Method
dvisc	0.0000635	Paxs	679.60	Joback Method
dvisc	0.0000415	Paxs	740.92	Joback Method
dvisc	0.0000290	Paxs	802.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378270&Units=SI
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

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
mccvol:	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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