Diethylmalonic acid, octyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C23H44O4/c1-8-11-12-13-14-15-16-26-20(24)23(9-2,10-3)21(25)27-18-19(4)17

InchiKey: SGJWOVFBDJTFSN-UHFFFAOYSA-N

Formula: C23H44O4

SMILES: CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	-321.82	kJ/mol	Joback Method
hf	-1030.43	kJ/mol	Joback Method
hfus	42.55	kJ/mol	Joback Method
hvap	82.12	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	6.312		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	924.99	kPa	Joback Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
tb	871.32	K	Joback Method
tc	1068.48	K	Joback Method
tf	483.13	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.56	J/mol×K	871.32	Joback Method
cpg	1240.53	J/mol×K	1035.62	Joback Method
cpg	1225.72	J/mol×K	1002.76	Joback Method
cpg	1209.88	J/mol×K	969.90	Joback Method
cpg	1192.94	J/mol×K	937.04	Joback Method
cpg	1174.86	J/mol×K	904.18	Joback Method
cpg	1254.37	J/mol×K	1068.48	Joback Method
dvisc	0.0000192	Pa×s	871.32	Joback Method

dvisc	0.0000271	Pa×s	806.62	Joback Method
dvisc	0.0000405	Pa×s	741.92	Joback Method
dvisc	0.0000656	Pa×s	677.22	Joback Method
dvisc	0.0001173	Pa×s	612.53	Joback Method
dvisc	0.0002409	Pa×s	547.83	Joback Method
dvisc	0.0005997	Pa×s	483.13	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=U369480&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