Azelaic acid, bis(2,2,4-trimethyl pentyl) ester

Inchi: InChI=1S/C25H48O4/c1-20(2)16-24(5,6)18-28-22(26)14-12-10-9-11-13-15-23(27)29-19-
InchiKey: RCVKOPJDEMAVNV-UHFFFAOYSA-N
Formula: C25H48O4
SMILES: CC(C)CC(C)(C)COC(=O)CCCCCCCC(=O)OCC(C)(C)CC(C)C
Mol. weight [g/mol]: 412.65
CAS: 1931-83-5

Physical Properties

Property code	Value	Unit	Source
gf	-307.42	kJ/mol	Joback Method
hf	-1076.99	kJ/mol	Joback Method
hfus	44.21	kJ/mol	Joback Method
hvap	86.19	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.948		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
tb	916.64	K	Joback Method
tc	1122.27	K	Joback Method
tf	490.67	K	Joback Method
vc	1.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.78	J/mol×K	916.64	Joback Method
cpg	1301.79	J/mol×K	950.91	Joback Method
cpg	1320.47	J/mol×K	985.18	Joback Method
cpg	1337.89	J/mol×K	1019.46	Joback Method
cpg	1354.12	J/mol×K	1053.73	Joback Method
cpg	1369.25	J/mol×K	1088.00	Joback Method
cpg	1383.33	J/mol×K	1122.27	Joback Method
dvisc	0.0005322	Pa×s	490.67	Joback Method
dvisc	0.0001920	Pa×s	561.66	Joback Method

dvisc	0.0000871	Pa×s	632.66	Joback Method
dvisc	0.0000463	Pa×s	703.65	Joback Method
dvisc	0.0000277	Pa×s	774.65	Joback Method
dvisc	0.0000180	Pa×s	845.64	Joback Method
dvisc	0.0000125	Pa×s	916.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1931835&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume