Eicosyl 3,3-dimethylbutanoate

Inchi: InChI=1S/C26H52O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-28-25(2
InchiKey: OJYAOFRTARGCDD-UHFFFAOYSA-N
Formula: C26H52O2
SMILES: CCCCCCCCCCCCCCCCCCCCCOC(=O)CC(C)(C)C
Mol. weight [g/mol]: 396.69

Physical Properties

Property code	Value	Unit	Source
gf	-63.04	kJ/mol	Joback Method
hf	-833.52	kJ/mol	Joback Method
hfus	58.47	kJ/mol	Joback Method
hvap	81.33	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	9.008		Crippen Method
mcvol	384.640	ml/mol	McGowan Method
pc	751.02	kPa	Joback Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tb	867.34	K	Joback Method
tc	1062.10	K	Joback Method
tf	457.36	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.38	J/mol×K	867.34	Joback Method
cpg	1307.91	J/mol×K	899.80	Joback Method
cpg	1329.17	J/mol×K	932.26	Joback Method
cpg	1349.20	J/mol×K	964.72	Joback Method
cpg	1368.09	J/mol×K	997.18	Joback Method
cpg	1385.89	J/mol×K	1029.64	Joback Method
cpg	1402.66	J/mol×K	1062.10	Joback Method
dvisc	0.0007919	Pa×s	457.36	Joback Method

dvisc	0.0003041	Pa×s	525.69	Joback Method
dvisc	0.0001456	Pa×s	594.02	Joback Method
dvisc	0.0000811	Pa×s	662.35	Joback Method
dvisc	0.0000504	Pa×s	730.68	Joback Method
dvisc	0.0000340	Pa×s	799.01	Joback Method
dvisc	0.0000244	Pa×s	867.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R399247&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

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