DIOCTYL AZELATE

Other names: Dioctyl nonanedioate
dioctyl azelate
Inchi: InChI=1S/C25H48O4/c1-3-5-7-9-14-18-22-28-24(26)20-16-12-11-13-17-21-25(27)29-23-
InchiKey: XWVQUJDBOICHGH-UHFFFAOYSA-N
Formula: C25H48O4
SMILES: CCCCCCCCOC(=O)CCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
af	1.2261		Cheméo Relay (1.0)
hf	-1167.57	kJ/mol	Cheméo Relay (1.0)
hfus	66.08	kJ/mol	Joback Method
hvap	116.11	kJ/mol	Cheméo Relay (1.0)
ie	9.57	eV	Cheméo Relay (1.0)
log10ws	-6.78		Cheméo Relay (1.0)
logp	7.524		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	804.33	kPa	Joback Method
tb	644.58	K	Cheméo Relay (1.0)
tc	815.06	K	Cheméo Relay (1.0)
tf	304.46	K	Cheméo Relay (1.0)
vc	1.479	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1370.09	J/mol×K	1099.83	Joback Method
cpg	1383.60	J/mol×K	1135.00	Joback Method
cpg	1301.94	J/mol×K	959.15	Joback Method
cpg	1321.17	J/mol×K	994.32	Joback Method
cpg	1338.92	J/mol×K	1029.49	Joback Method
cpg	1355.21	J/mol×K	1064.66	Joback Method
cpg	1281.17	J/mol×K	923.98	Joback Method

dvisc	0.0001173	Pa×s	651.88	Joback Method
dvisc	0.0002153	Pa×s	583.85	Joback Method
dvisc	0.0004642	Pa×s	515.83	Joback Method
dvisc	0.0000716	Pa×s	719.90	Joback Method
dvisc	0.0000476	Pa×s	787.93	Joback Method
dvisc	0.0000338	Pa×s	855.96	Joback Method
dvisc	0.0000252	Pa×s	923.98	Joback Method
hvapt	104.30	kJ/mol	458.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2064804&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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