

Isophthalic acid, decyl 2-methylcyclohexyl ester

Inchi:	InChI=1S/C25H38O4/c1-3-4-5-6-7-8-9-12-18-28-24(26)21-15-13-16-22(19-21)25(27)29-2
InchiKey:	IKESYGHOWXFUSS-UHFFFAOYSA-N
Formula:	C25H38O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OC2CCCCC2C)c1
Mol. weight [g/mol]:	402.57

Physical Properties

Property code	Value	Unit	Source
gf	-188.70	kJ/mol	Joback Method
hf	-789.89	kJ/mol	Joback Method
hfus	52.64	kJ/mol	Joback Method
hvap	92.61	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	6.720		Crippen Method
mvol	343.370	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
rinpol	3089.00		NIST Webbook
rinpol	3089.00		NIST Webbook
tb	970.52	K	Joback Method
tc	1191.66	K	Joback Method
tf	557.91	K	Joback Method
vc	1.308	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.70	J/molxK	970.52	Joback Method
cpg	1197.54	J/molxK	1007.38	Joback Method
cpg	1212.63	J/molxK	1044.23	Joback Method
cpg	1226.02	J/molxK	1081.09	Joback Method
cpg	1237.75	J/molxK	1117.95	Joback Method
cpg	1247.86	J/molxK	1154.81	Joback Method
cpg	1256.40	J/molxK	1191.66	Joback Method
dvisc	0.0004367	Paxs	557.91	Joback Method

dvisc	0.0002300	Paxs	626.68	Joback Method
dvisc	0.0001375	Paxs	695.45	Joback Method
dvisc	0.0000902	Paxs	764.21	Joback Method
dvisc	0.0000634	Paxs	832.98	Joback Method
dvisc	0.0000471	Paxs	901.75	Joback Method
dvisc	0.0000364	Paxs	970.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U345754&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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

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